Supporting Information

Donor-Modified Multiple Resonance Emitters with Accelerated Reverse Intersystem Crossing towards High-Efficiency and Narrowband Deep-Blue OLEDs

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General Information

All reagents and solvents were purchased from commercial sources and used without further purification. All reactions were performed under argon conditions using anhydrous solvents. The final products were first purified by column chromatography, and then further refined by sublimation. ^{1}H NMR (500 MHz), ^{13}C NMR (125 MHz) spectra were recorded on Bruker AV 500 NMR instrument at ambient temperature using deuterated solvents. Chemical shifts were given parts per million (ppm) relative to tetramethyl silane (δ = 0 ppm). High-resolution mass spectra (HRMS) were measured on a Bruker maxis UHR-TOF mass spectrometer. Elemental analysis (EA) was performed on Elemantar: Vario EL cube lemantar. Thermogravimetric analysis (TGA) was undertaken using TGA-Q50 Instrument (TA Instrument, American) at a heating of 10 °C/min from 30 °C to 800 °C under nitrogen flushing. The thermal decomposition temperature (T_d) was determined by the recorded temperature at 5% weight loss. Differential scanning calorimetry (DSC) was performed at a heating of 10 °C/min from 30 °C to 300 °C using a TA DSC-Q200 (TA Instrument, American) under nitrogen condition, and T_g was determined from the second heating scan. Cyclic voltammetry (CV) measurements were carried out on a CHI600 electrochemical analyzer (Chenhua, China) at room temperature, with a conventional three-electrode system consisting of a glassy carbon working electrode, a platinum wire auxiliary electrode, and an Ag/AgCl standard electrode using as the reference electrode. The supporting electrolyte was 0.1 M tetrabutylammonium hexafluorophosphate ($^{t}Bu_4NPF_6$) in anhydrous dichloromethane solution, and ferrocene was added as a calibrant in the whole measurement. The HOMO energy levels of the compounds were calculated according to the formula: E_{HOMO} (eV) = -[4.8 + ($E_{1/2}$(ox/red) - $E_{1/2}$(Fc+/Fc))] eV. The LUMO energy levels of the compounds were deduced from the HOMO levels and the UV-vis absorption onsets of the longer wavelength.

Synthesis

Synthesis of 2,5-dibromo-1-(4-(tert-butyl)phenoxy)-3-fluorobenzene (**2**): A mixture of 2,5-dibromo-1,3-difluorobenzene (12.00 g, 44.13 mmol), 4-tert-Butylphenol (7.95 g, 52.95 mmol) and K_2CO_3 (12.21 g, 88.26 mmol) in N,N-Dimethylformamide (70 mL) was stirred at 90 ºC for 12 h under argon atmosphere. After cooling to room temperature, the mixture was diluted with dichloromethane and then added into water. The organic layer was separated and the aqueous layer was extracted with dichloromethane three times. The combined organic fractions were dried over anhydrous Na_2SO_4 and the solvent was removed under vacuum. The crude product was purified by silica gel chromatography using petroleum ether/dichloromethane (10/1,

v/v) as eluent to give the intermediate **2** as a white solid (12.78 g, 72%). ^{1}H NMR (500 MHz, $CDCl_3$): δ (ppm) 7.40 (d, J = 8.7 Hz, 2H), 7.04 (dd, J = 7.6, 2.0 Hz, 1H), 6.96 (d, J = 8.7 Hz, 2H), 6.77 (t, J = 1.6 Hz, 1H), 1.34 (s, 9H).

Synthesis of 3,6-di-tert-butyl-9-(2,5-dibromo-3-(4-(tert-butyl)phenoxy)phenyl)-9H-carbazole (**3**): A mixture of **2** (12.00 g, 29.85 mmol), 3,6-di-tert-butyl-9*H*-carbazole (9.75 g, 35.82 mmol) and Cs_2CO_3 (19.44 g, 35.70 mmol) in N,N-Dimethylformamide (70 mL) was stirred at 155 ºC for 12 h under argon atmosphere. After cooling to room temperature, the crude product was removed under vacuum and then purified by silica gel chromatography using petroleum ether/dichloromethane (5/1, v/v) as eluent to give the intermediate **3** as a white solid (13.98 g, 71%). ^{1}H NMR (600 MHz, $CDCl_3$): δ (ppm) 8.14 (s, 2H), 7.47 (t, J = 9.0 Hz, 4H), 7.32 (d, J = 1.8 Hz, 1H), 7.12 (d, J = 2.0 Hz, 1H), 7.07 (dd, J = 8.6, 3.7 Hz, 4H), 1.47 (s, 18H), 1.37 (s, 9H).

Synthesis of 7-bromo-2,11,14-tri-tert-butyl-5-oxa-8b-aza-15b-borabenzo[a]naphtho[1,2,3-hi]aceanthrylene (**BNO-Br**): A solution of *n*-butyllithium in hexane (7.4 ml, 2.5 M, 18.56 mmol) was added slowly to a solution of **3** (11.20 g, 16.96 mmol) in anhydrous 1,2-dichlorobenzene (70 mL) at -40 ºC under argon atmosphere. The mixture was stirred at room temperature for 1 h. Then boron tribromide (8.48 g, 3.28 mL, 33.84 mmol) was added slowly at 0 ºC and stirred at room temperature for 2 h. Then *N,N*-diisopropylethylamine (DIPEA, 4.4 g, 5.6 mL, 33.84 mmol) was added at 0 ºC and kept at room temperature for 15 min. The reaction mixture was then stirred at 140 ºC for 16 h. After cooling to room temperature, the reaction mixture was filtered, and the residue was washed with ethanol to afford the desired compound BNO-Br as a yellow solid (7.00 g, 70%). ^{1}H NMR (500 MHz, $CDCl_3$): δ (ppm) 8.94-8.92 (m, 1H), 8.84 (d, J = 2.2 Hz, 1H), 8.45-8.42 (m, 1H), 8.23-8.16 (m, 3H), 7.76 (dd, J = 8.7, 2.3 Hz, 1H), 7.65 (dd, J = 8.7, 1.7 Hz, 1H), 7.44 (d, J = 8.7 Hz, 1H), 7.36 (s, 1H), 1.63 (s, 9H), 1.52 (s, 18H).

Synthesis of 2,11,14-tri-tert-butyl-7-(9,9-diphenylacridin-10(9H)-yl)-5-oxa-8b-aza-15b-borabenzo[a]naphtho[1,2,3-hi]aceanthrylene **(BNO-DPAC):** BNO-Br (0.74 g, 1.25 mmol), 9,9-diphenyl-9,10-dihydroacridine (0.51 g, 1.51 mmol), $Pd(OAc)_2$ (14 mg, 0.063 mmol),^{t}Bu$_3$PHBF$_4$ (55 mg, 0.189 mmol),and NaO^{t}Bu (0.37 g, 3.78 mmol) were added into a 100 mL two neck flask. After that, 25 mL toluene was injected into the two-neck flask under argon atmosphere. The mixture was stirred at 110 ºC for 18 h. After cooling to room temperature, the crude product was removed under vacuum and then purified by silica gel chromatography using petroleum ether/dichloromethane (9/1, v/v) as eluent to give the product **BNO-DPAC**

as yellow powder. The powder was further purified by sublimation to afford the product as greenish yellow crystal (0.57 g, 45%). ^{1}H NMR (500 MHz, $CDCl_3$): δ (ppm) 9.01 (d, J = 1.6 Hz, 1H), 8.93 (d, J = 2.3 Hz, 1H), 8.47 (d, J = 1.6 Hz, 1H), 8.20 (d, J = 1.8 Hz, 1H), 7.80 (dd, J = 8.8, 2.3 Hz, 1H), 7.77-7.74 (m, 1H), 7.66 (d, J = 8.8 Hz, 1H), 7.52-7.48 (m, 2H), 7.35 (dd, J = 5.2, 1.6 Hz, 6H), 7.19-7.18 (m, 1H), 7.11-7.06 (m, 6H), 6.98-6.92 (m, 4H), 6.74 (d, J = 8.0 Hz, 2H), 1.64 (s, 9H), 1.54 (s, 9H), 1.49 (s, 9H). ^{13}C NMR (125 MHz, $CDCl_3$): δ (ppm) 157.98, 146.51, 145.92, 145.43, 145.14, 144.22, 142.08, 137.99, 131.50, 130.80, 130.67, 130.30, 130.07, 129.74, 127.89, 127.24, 126.46, 124.81, 121.47, 120.64, 117.60, 117.20, 114.56, 114.17, 111.61, 109.58, 57.13, 35.33, 34.90, 34.77, 32.28, 31.92, 31.76. HRMS: (ESI) m/z calcd for $C_{61}H_{55}BN_2O$ [M^+]: 843.44802; Found: 843.44769. Elemental analysis calcd. (%) for $C_{61}H_{55}BN_2O$: C, 86.92; H, 6.58; N, 3.32. Found: C, 86.07; H, 6.20; N, 3.30.

Synthesis of 2,11,14-tri-tert-butyl-7-(9,9-dimethylacridin-10(9H)-yl)-5-oxa-8b-aza-15b-borabenzo[a]naphtho[1,2,3-hi]aceanthrylene **(BNO-DMAC):** Compound **BNO-DMAC** was synthesized according to the procedure of **BNO-DPAC** in which 9,9-dimethyl-9,10-dihydroacridine was used as the substrate instead of 9,9-diphenyl-9,10-dihydroacridine. The crude product was removed under vacuum and then purified by silica gel chromatography using petroleum ether as eluent to give the product **BNO-DMAC** as yellow powder. The powder was further purified by sublimation to afford the product as greenish yellow solid (0.25 g, 45%). ^{1}H NMR (400 MHz, $CDCl_3$): δ (ppm) 9.03 (d, J = 1.6 Hz, 1H), 8.94 (d, J = 2.3 Hz, 1H), 8.49 (d, J = 1.6 Hz, 1H), 8.22 (d, J = 1.8 Hz, 1H), 8.19-8.15 (m, 1H), 8.10 (d, J = 8.8 Hz, 1H), 7.80 (dd, J = 8.7, 2.4 Hz, 1H), 7.55-7.49 (m, 4H), 7.30 (d, J = 1.1 Hz, 1H), 6.98 (ddt, J = 9.7, 7.1, 3.5 Hz, 4H), 6.61-6.54 (m, 2H), 1.78 (s, 6H), 1.66 (s, 9H), 1.54 (s, 9H), 1.46 (s, 9H). ^{13}C NMR (125 MHz, $CDCl_3$): δ (ppm) 161.43, 158.03, 146.80, 145.90, 145.42, 145.19, 144.33, 142.31, 140.82, 138.08, 131.48, 130.79, 130.76, 129.77, 126.94, 126.71, 125.42, 124.91, 124.32, 121.49, 121.14, 117.63, 117.30, 114.90, 114.14, 110.93, 109.46, 36.33, 35.34, 34.92, 34.78, 32.29, 31.89, 31.77, 31.42. HRMS: (ESI) m/z calcd for $C_{51}H_{51}BN_2O$ [M^+]: 719.41672; Found: 719.41742. Elemental analysis calcd. (%) for $C_{51}H_{51}BN_2O$: C, 85.22; H, 7.15; N, 3.90. Found: C, 84.63; H, 6.80; N, 3.86.

Synthesis of 2,11,14-tri-tert-butyl-7-(2,7-di-tert-butyl-9,9-dimethylacridin-10(9H)-yl)-5-oxa-8b-aza-15b-borabenzo[a]naphtho[1,2,3-hi]aceanthrylene **(BNO-*t*BuDMAC):** Compound **BNO-*t*BuDMAC** was synthesized according to the procedure of **BNO-DPAC** in which 2,7-di-tert-butyl-9,9-dimethyl-9,10-

dihydroacridine was used as the substrate instead of 9,9-diphenyl-9,10-dihydroacridine. The crude product was removed under vacuum and then purified by silica gel chromatography using petroleum ether as eluent to give the product **BNO-*t*BuDMAC** as yellow powder. The powder was further purified by sublimation to afford the product as greenish yellow solid (0.33 g, 52%). ^{1}H NMR (400 MHz, $CDCl_3$): δ (ppm) 9.03 (d, J = 1.7 Hz, 1H), 8.93 (d, J = 2.4 Hz, 1H), 8.48 (d, J = 1.7 Hz, 1H), 8.22 (s, 1H), 8.16 (d, J = 1.3 Hz, 1H), 8.09 (d, J = 8.8 Hz, 1H), 7.78 (d, J = 2.4 Hz, 1H), 7.54 (d, J = 2.2 Hz, 2H), 7.53-7.48 (m, 2H), 7.29 (s, 1H), 7.05 (d, J = 2.2 Hz, 1H), 7.03 (d, J = 2.2 Hz, 1H), 6.59 (s, 1H), 6.57 (s, 1H), 1.79 (s, 6H), 1.66 (s, 9H), 1.54 (s, 9H), 1.47 (s, 9H), 1.33 (s, 18H). ^{13}C NMR (125 MHz, $CDCl_3$): δ (ppm) 161.36, 158.06, 147.59, 145.76, 145.28, 145.06, 144.18, 143.75, 142.33, 138.68, 138.09, 131.34, 131.20, 130.76, 129.73, 126.91, 124.76, 124.25, 123.46, 122.22, 121.34, 117.61, 117.25, 115.13, 114.21, 109.63, 108.38, 36.93, 35.34, 34.91, 34.77, 34.47, 32.30, 31.90, 31.78, 31.71, 31.43. HRMS: (ESI) m/z calcd for $C_{59}H_{67}BN_2O$ [M^+]: 831.54302; Found: 831.54272. Elemental analysis calcd. (%) for $C_{59}H_{67}BN_2O$: C, 85.28; H, 8.13; N, 3.37. Found: C, 84.78; H, 7.67; N, 3.37.

Quantum Chemical Calculations

All of the simulation calculations were carried out with Gaussian 09 program package. Density functional theory (DFT) calculations on the geometrical and electronic properties of the ground-state were performed based on B3LYP-D3(BJ) hybrid functional with m062x/def2svp.

Photophysical Characterization

The UV-vis absorption spectra were obtained on a Shimadzu UV-2600 spectrophotometer (Shimadzu, Japan) at room temperature with a concentration of 1×10^{-5} M. Phosphorescence spectra were measured on a Hitachi F-7100 fluorescence spectrophotometer at 77 K. The transient photoluminescence (PL) decay curves were obtained by FluoTime 300 (PicoQuant GmbH) with a Picosecond Pulsed UV-LASTER (LASTER375) as the excitation source. The solid-state PL quantum efficiencies (Φ_{PL}s) were measured on a Hamamatsu UV-NIR absolute PL quantum yield spectrometer (C13534, Hamamatsu Photonics) equipped with an integrating sphere. The integrating sphere was purged with dry argon to maintain an inert atmosphere and all the samples were excited at 320 nm. Nanosecond time-resolved transient absorption spectra and decay kinetics were measured on LFP instrument (LP 980, Edinburgh Instruments Ltd). The pump laser beam and the probe beam crossed perpendicularly through the liquid sample in a quartz cuvette (10 mm × 10 mm). A dynamic decay

curve was recorded with a digital phosphor oscilloscope (TDS 3012C, Tektronix Inc.).

Single Crystal X-ray Crystallographic Data

The single crystals of the new emitters were prepared from ethanol/dichloromethane mixtures by slow solvent evaporation and then subjected to crystallography analysis. X-ray single crystal data of **BNP-DPAC** and **BNO-*t*BuDMAC** were collected on a Bruker D8 Venture diffractometer using MoK radiation (λ = 0.71073) source. The selected crystal was kept at 150.0 K during data collection. Using Olex2[1], the structure was solved with the ShelXT[2] structure solution program using Intrinsic Phasing and refined with the ShelXL[3] refinement package using Least Squares minimization. Selected crystal data and experimental details are listed below. All crystallographic information in CIF format have been deposited at the Cambridge Crystallographic Data Center (CCDC) under deposition number 2270878 for **BNP-DPAC** and 2270880 for **BNO-*t*BuDMAC** via www.ccdc.cam.ac.uk/data_request/cif.

Analysis of Rate Constants

The rate constants of radiative decay ($k_{r,S}$) and nonradiative decay ($k_{nr,S}$) from S_1 to S_0 states, the rate constants of intersystem crossing (k_{ISC}) and reverse intersystem crossing (k_{RISC}) could be estimated using the following equations.[4-6]

$$k_{r,S} = \Phi_p k_p + \Phi_d k_d \approx \Phi_p k_p \quad \text{Eq.(1)}$$

$$k_{nr,S} = \frac{1 - \Phi_{PL}}{\Phi_{PL}} k_{r,S} \quad \text{Eq.(2)}$$

$$k_{ISC} = k_p - k_{r,S} - k_{nr,S} \quad \text{Eq.(3)}$$

$$k_{RISC} = (k_p k_d \Phi_d)/(k_{ISC} \Phi_p) \quad \text{Eq.(4)}$$

Where k_p and k_d represent the decay rate constants for prompt and delayed fluorescence, respectively, which are in reciprocal relationship with the decay time constants (τ_p and τ_d) experimentally determined from transient PL characteristics. Φ_p and Φ_d indicate prompt and delayed fluorescence components and can be distinguished from the total Φ_{PL} by comparing the integrated intensities of prompt (r_p) and delayed components (r_d) in the transient PL spectra. r_p and r_d were determined using τ_p and τ_d and fitting parameter (A_p, A_d) as follows.

$$I(t) = A_p e^{-\frac{1}{\tau_p}} + A_d e^{-\frac{1}{\tau_d}} \quad \text{Eq.(5)}$$

$r_p = A_p\tau_p/(A_p\tau_p + A_d\tau_d)$ ……Eq.(6)

$r_d = A_d\tau_d/(A_p\tau_p + A_d\tau_d)$ ……Eq.(7)

Device Fabrication and Measurement

The optimized structure for hyperfluorescent (HF) device: (ITO)/HAT-CN (5 nm)/TAPC (30 nm)/TCTA (15 nm)/mCBP (10 nm)/ DBFPO:3Cz2BN (20 wt%):MR-TADF emitters (1 wt%) (EML, 25 nm)/DBFPO (20 nm)/ANT-BIZ (30 nm)/ Liq/Al.

Fabrication and measurement detail: The ITO coated glass substrates with a sheet resistance of 15 Ω square^{-1} were consecutively ultrasonicated with acetone/ethanol and dried with nitrogen gas flow, followed by 20 min ultraviolet light-ozone (UVO) treatment in a UV-ozone surface processor (PL16 series, Sen Lights Corporation). Then the sample was transferred to the deposition system. Both 8-hydroxyquinolinolato-lithium (Liq) as electron injection layer and aluminum (Al) as cathode layer were deposited by thermal evaporation at 5×10^{-5} Pa. The organic layers were deposited at the rates of 0.2-3 Å/s. After the organic film deposition, Liq and Al layer were deposited with rates of 0.1 and 3 Å/s, respectively. The emitting area of the device is about 0.09 cm^2. The current density-voltage-luminance (*J-V-L*), *L-EQE* curves and electroluminescence spectra were measured using a Keithley 2400 source meter and an absolute EQE measurement system (C9920-12, Hamamatsu Photonics, Japan).

Schemes, Fig.s and Tables

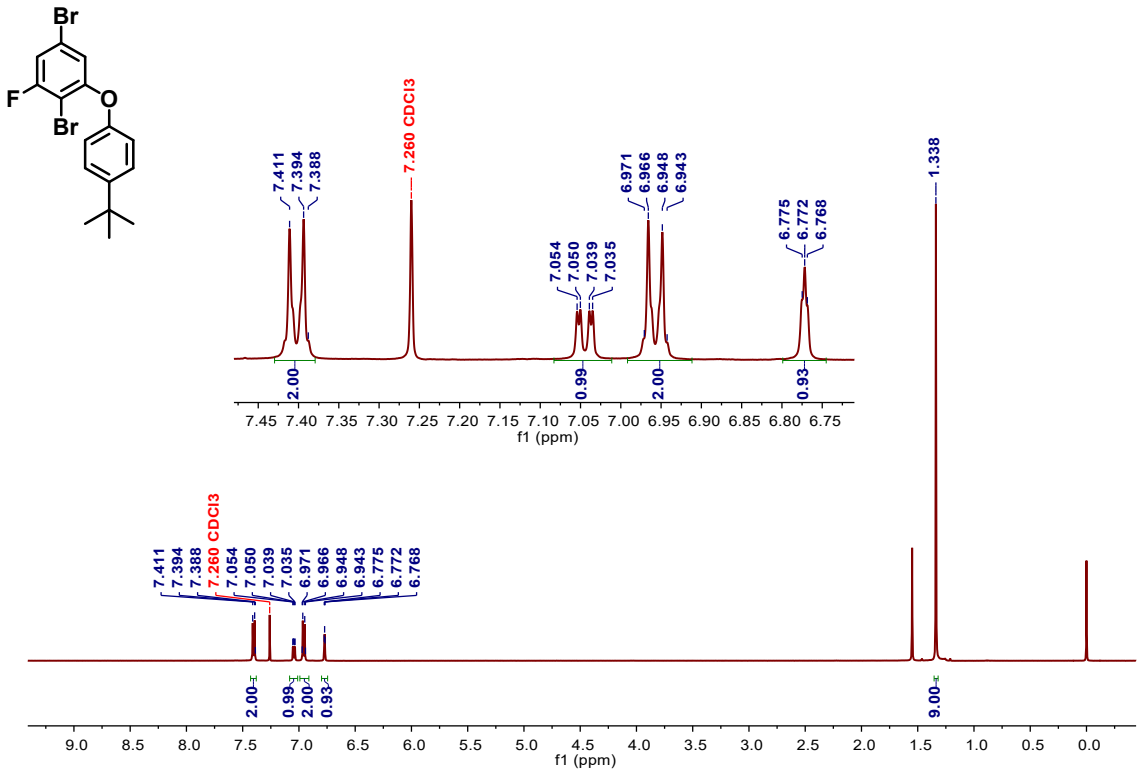


Fig. S1. ^{1}H NMR spectrum of **2** in $CDCl_3$ (500 MHz, 25 ^{o}C).

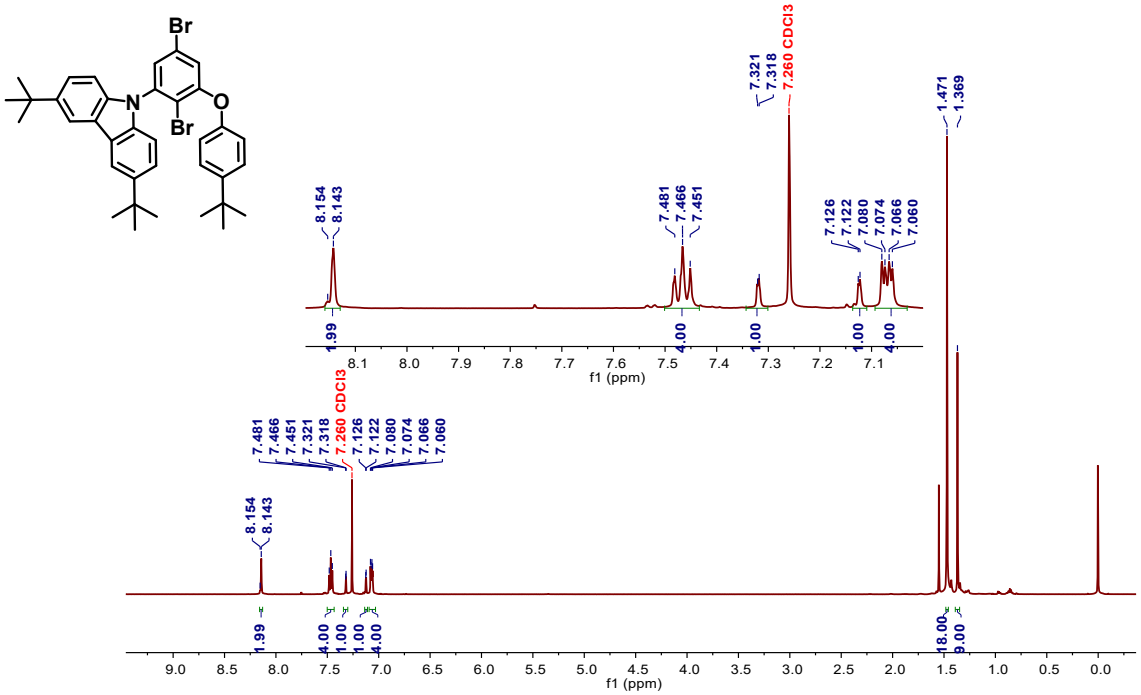


Fig. S2. ^{1}H NMR spectrum of **3** in $CDCl_3$ (500 MHz, 25 ^{o}C).

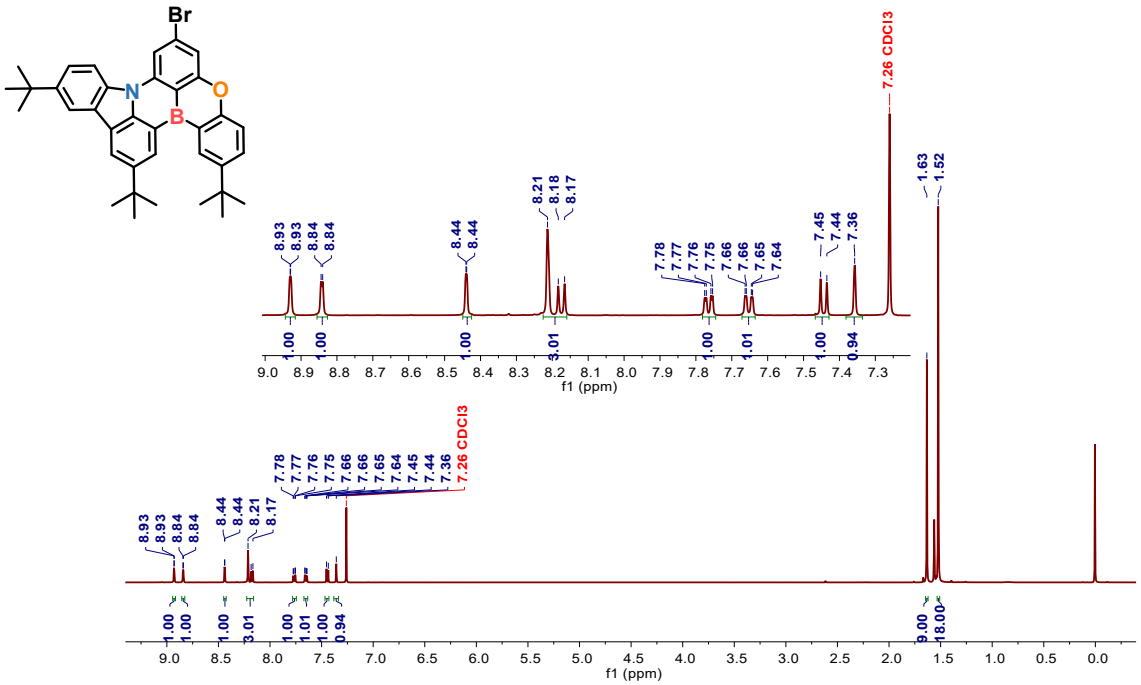


Fig. S3. ^{1}H NMR spectrum of **BNO-Br** in $CDCl_3$ (500 MHz, 25 °C).

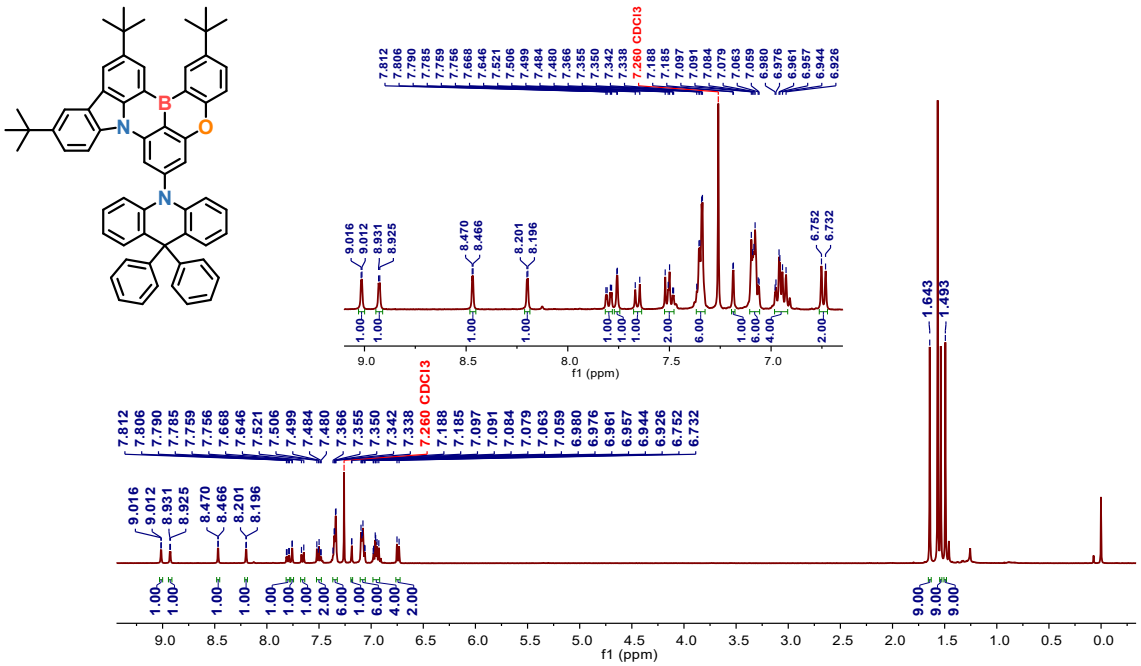


Fig. S4. ^{1}H NMR spectrum of **BNO-DPAC** in $CDCl_3$ (500 MHz, 25 °C).

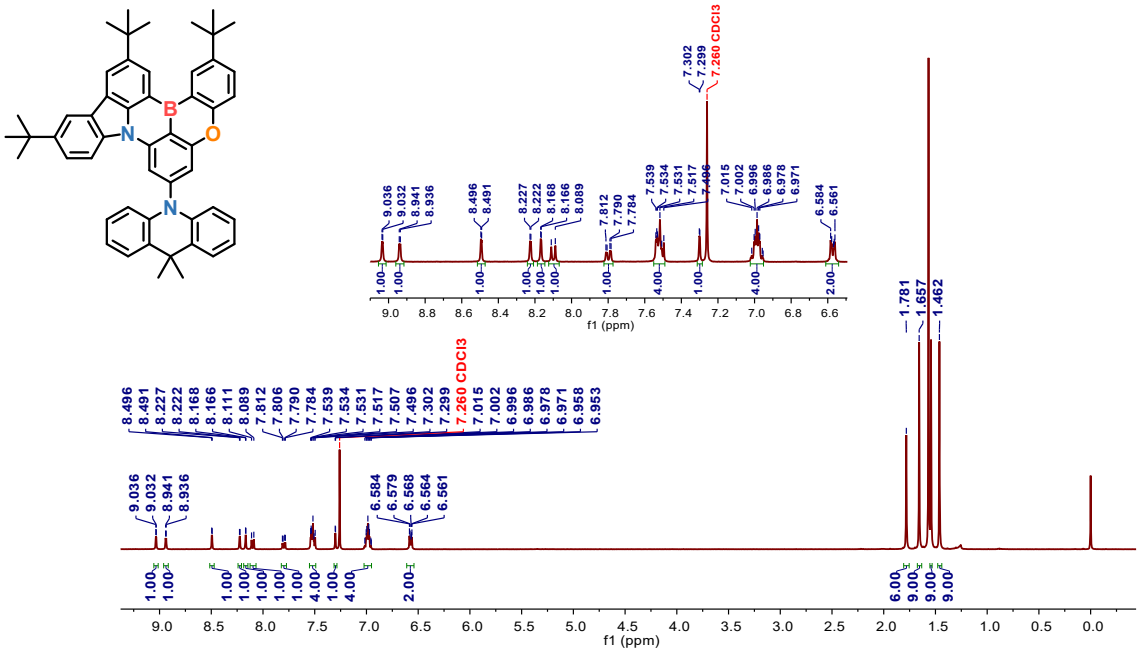


Fig. S5. ^{1}H NMR spectrum of **BNO-DMAC** in $CDCl_3$ (500 MHz, 25 °C).

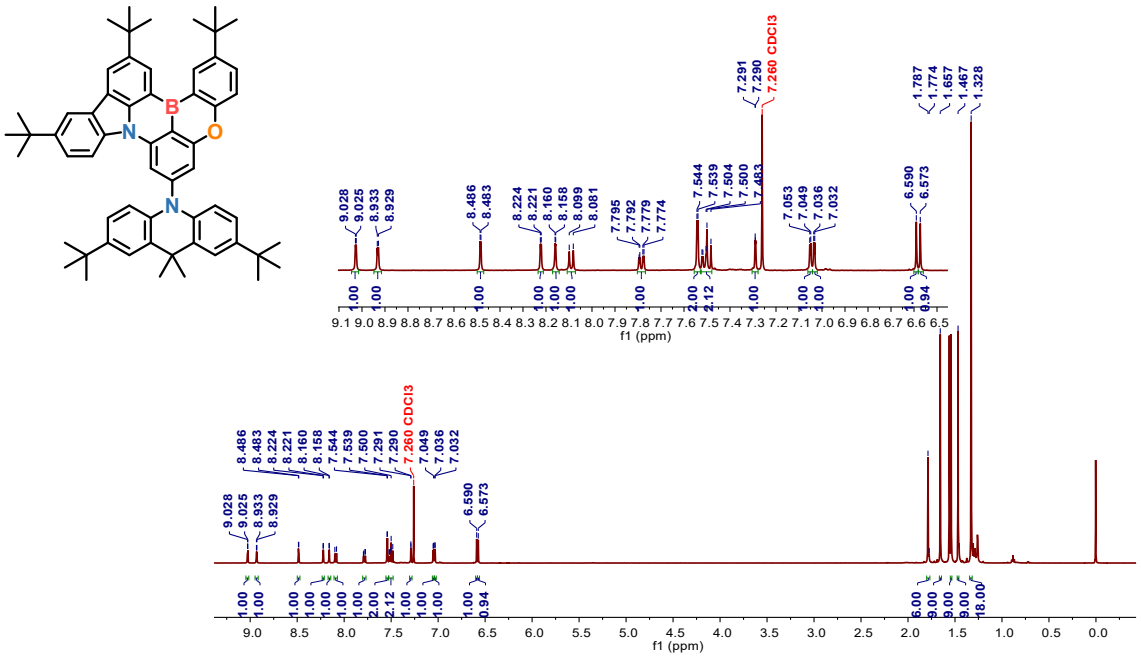


Fig. S6. ^{1}H NMR spectrum of **BNO-*t*BuDMAC** in $CDCl_3$ (500 MHz, 25 °C).

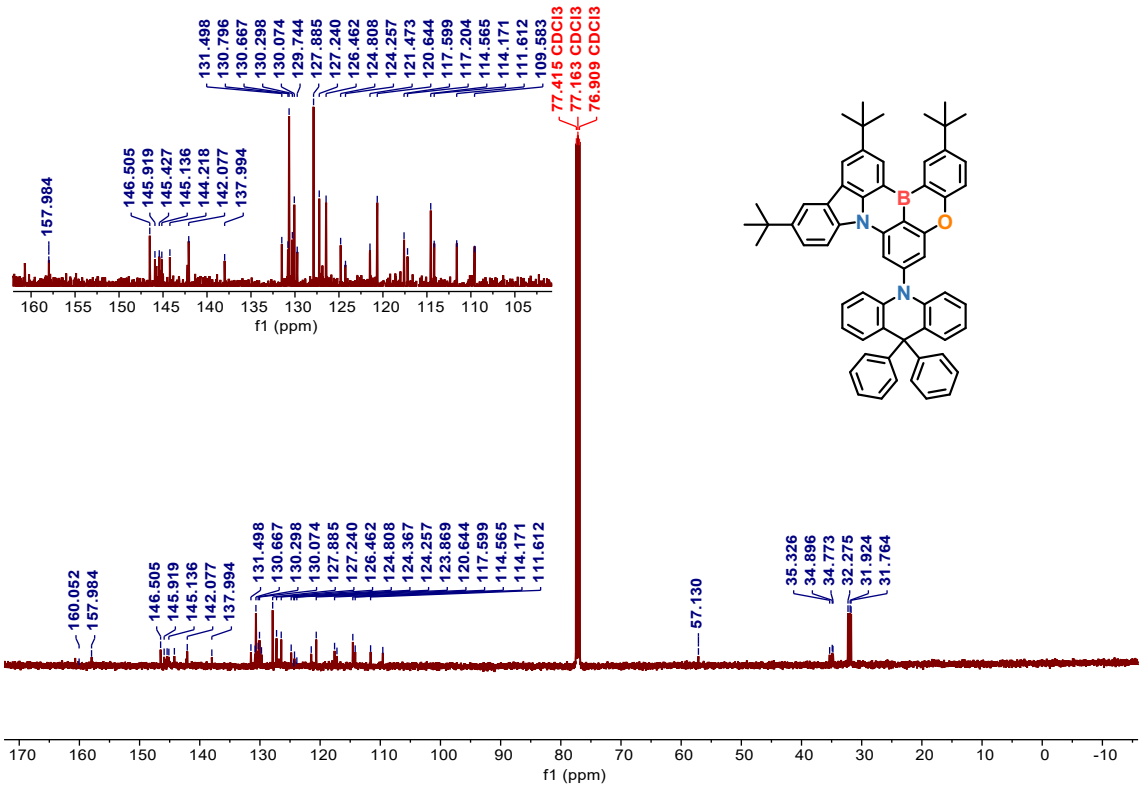


Fig. S7. ^{13}C NMR spectrum of **BNO-DPAC** in $CDCl_3$ (125 MHz, 25 °C).

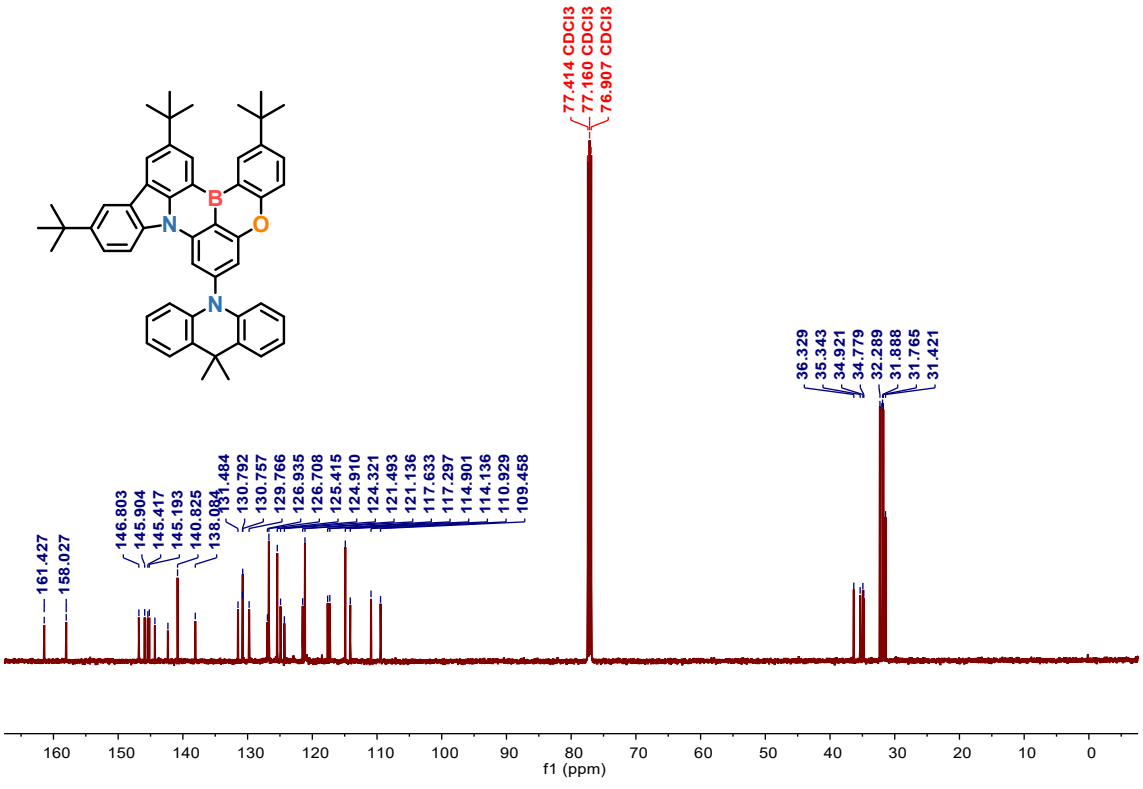


Fig. S8. ^{13}C NMR spectrum of **BNO-DMAC** in $CDCl_3$ (125 MHz, 25 °C).

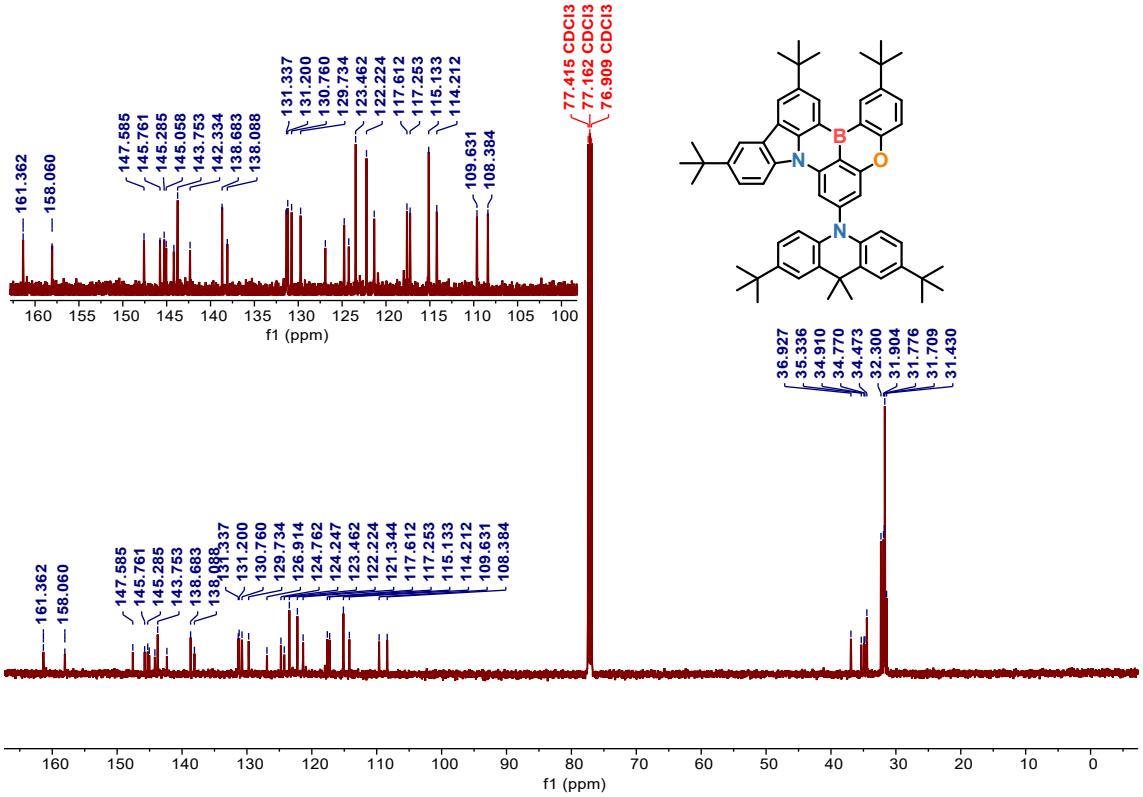


Fig. S9. ^{13}C NMR spectrum of **BNO-*t*BuDMAC** in $CDCl_3$ (125 MHz, 25 °C).

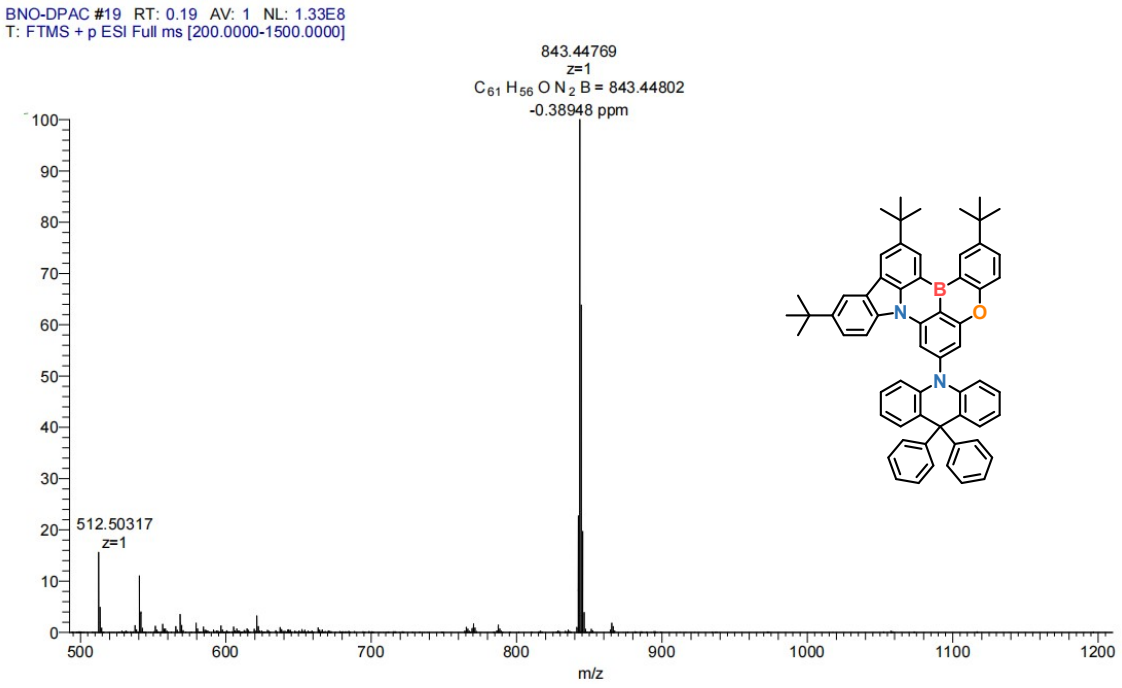


Fig. S10. HR-MS spectrum of **BNO-DPAC**.

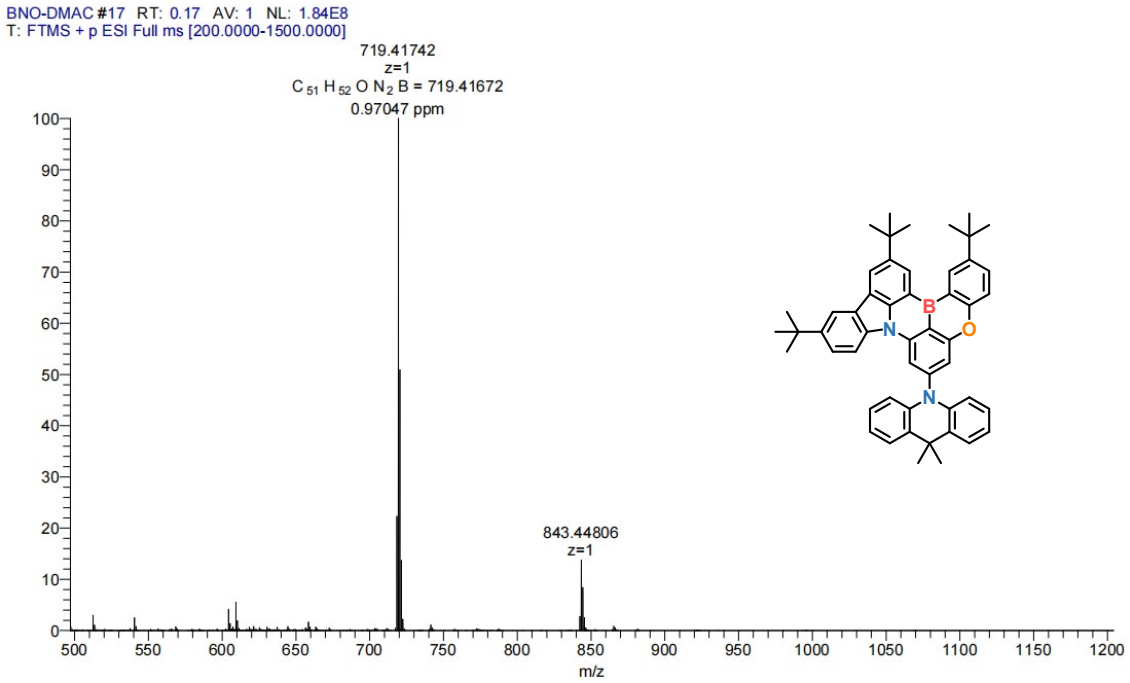


Fig. S11. HR-MS spectrum of **BNO-DMAC**.

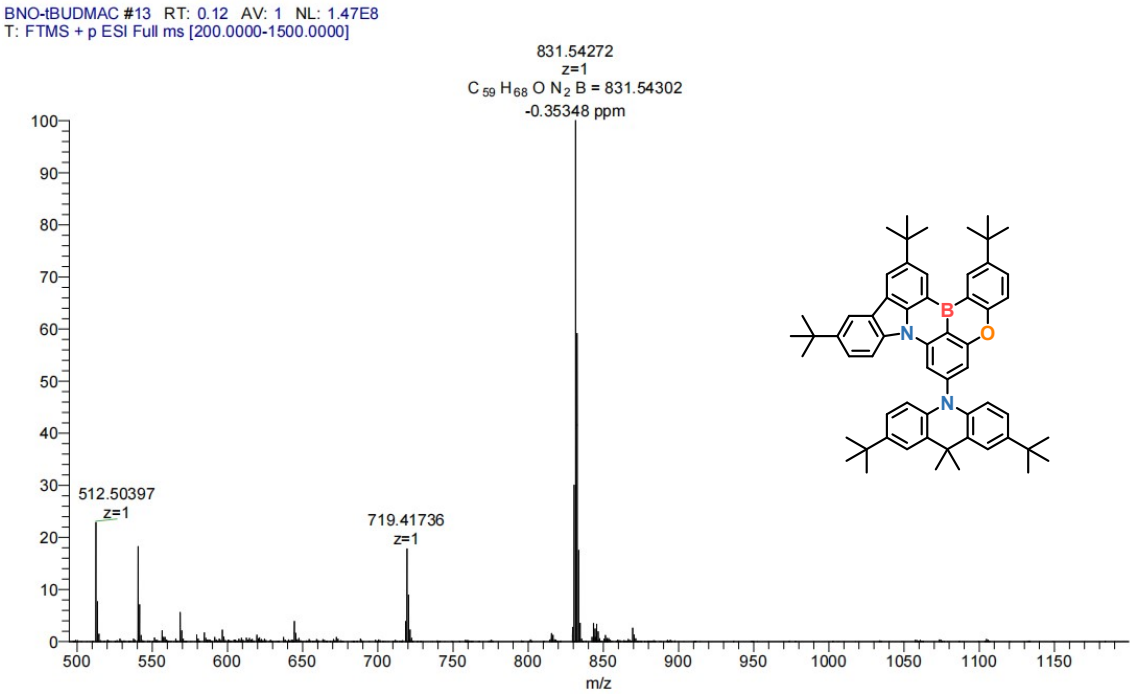
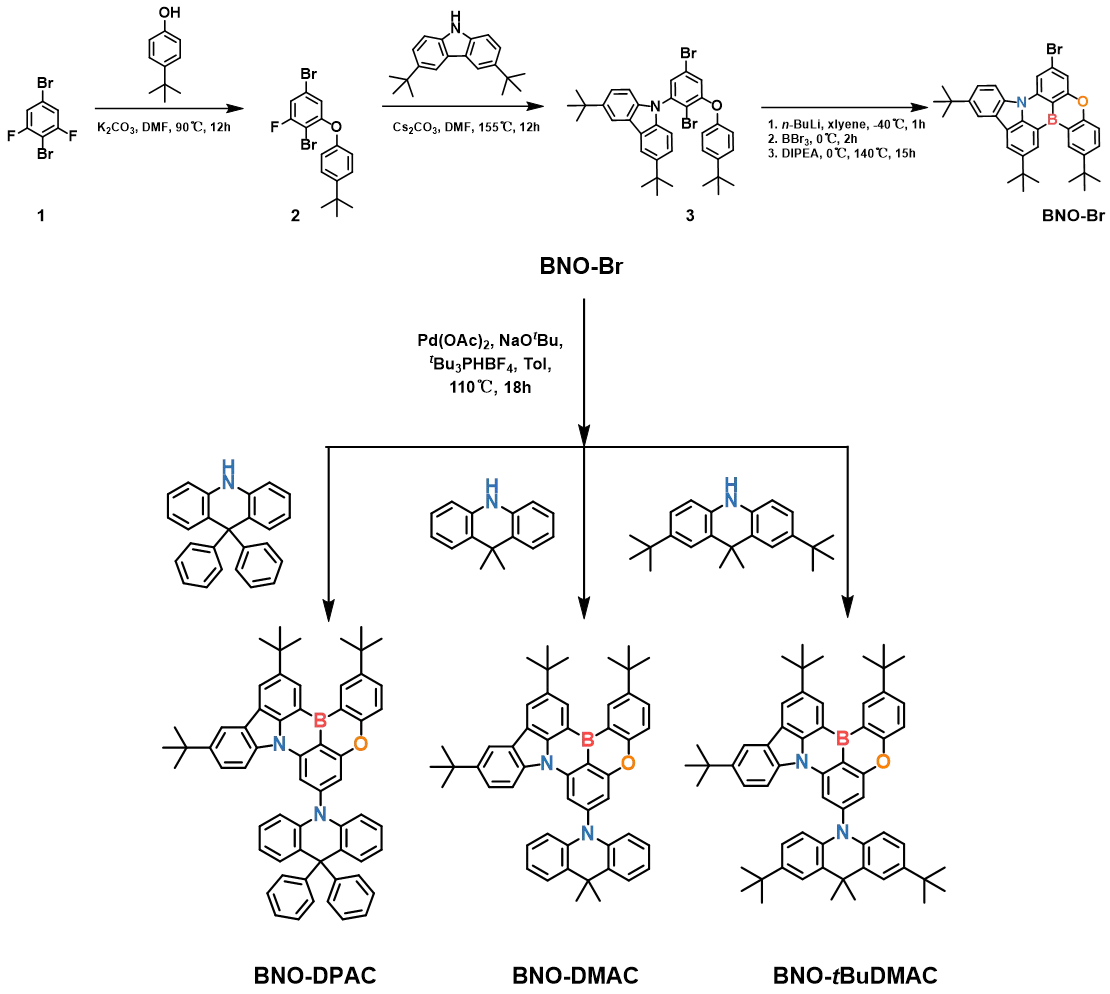


Fig. S12. HR-MS spectrum of **BNO-*t*BuDMAC**.



Scheme S1. The synthetic route of **BNO-DPAC**, **BNO-DMAC** and **BNO-*t*BuDMAC**.

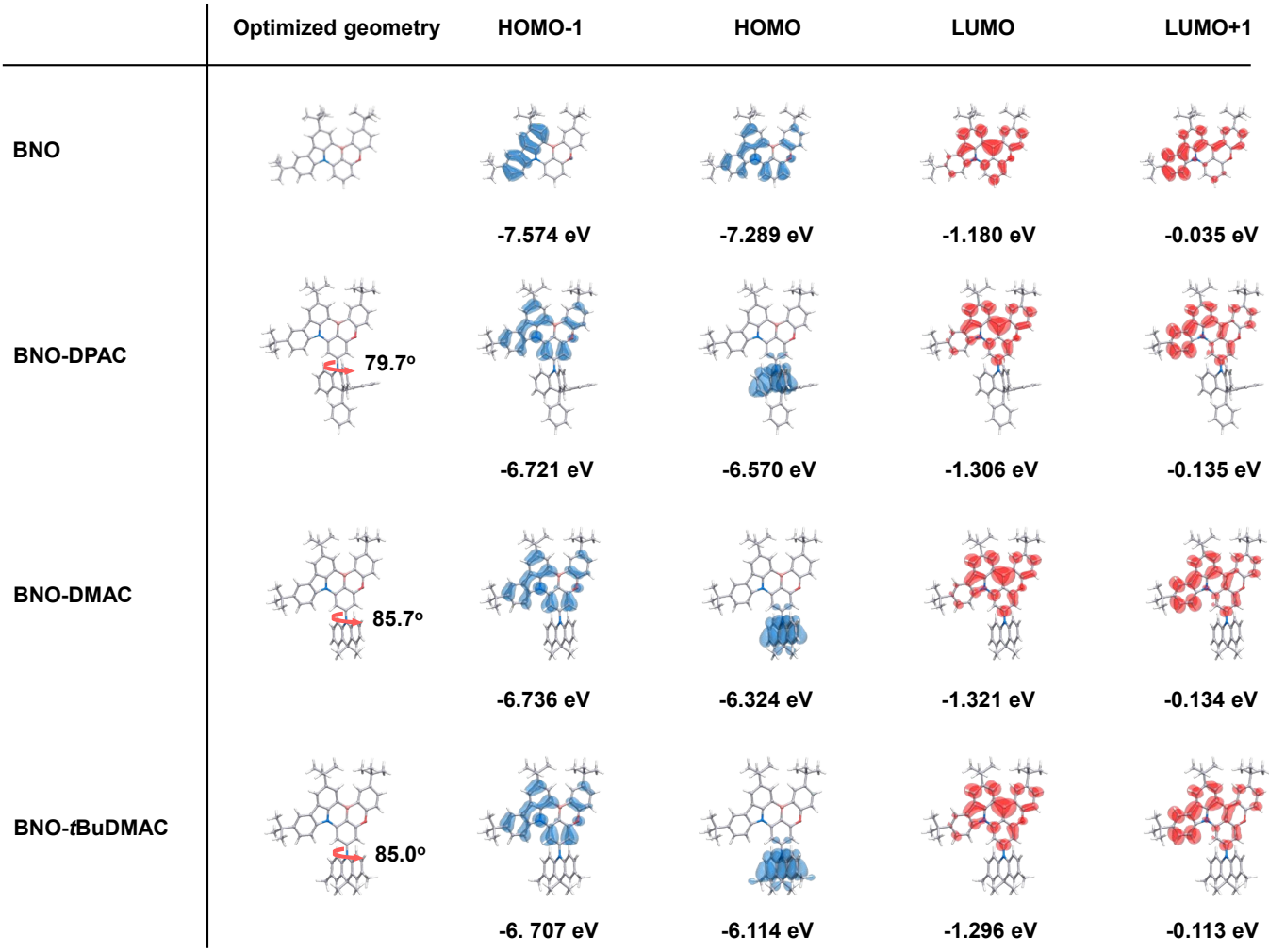


Fig. S13. The optimized geometries, frontier molecular orbital distributions (FMO) and related energy levels of (A) **BNO**, (B) **BNO-DPAC**, (C) **BNO-DMAC** and (D) **BNO-*t*BuDMAC**.

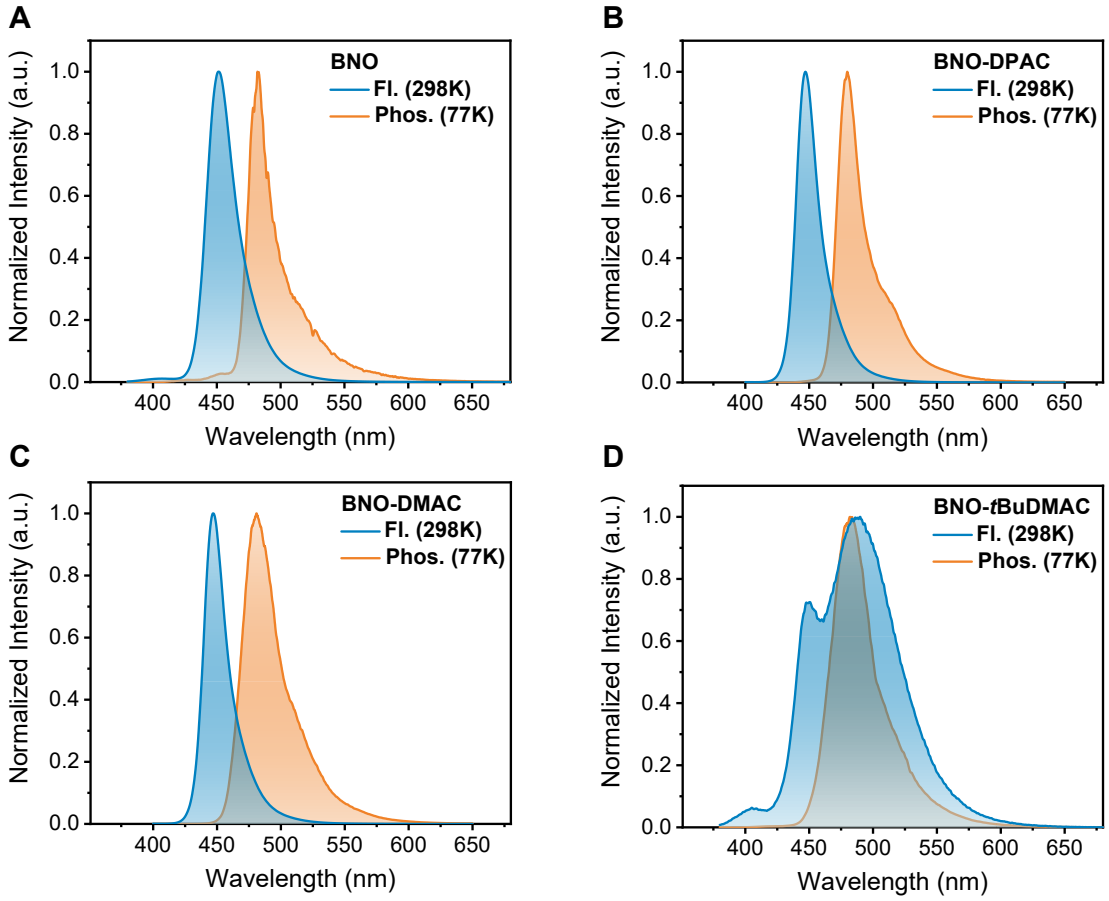


Fig. S14. Fluorescence and phosphorescence spectra of (A) **BNO**, (B) **BNO-DPAC**, (C) **BNO-DMAC** and (D) **BNO-*t*BuDMAC** in dilute toluene solution.

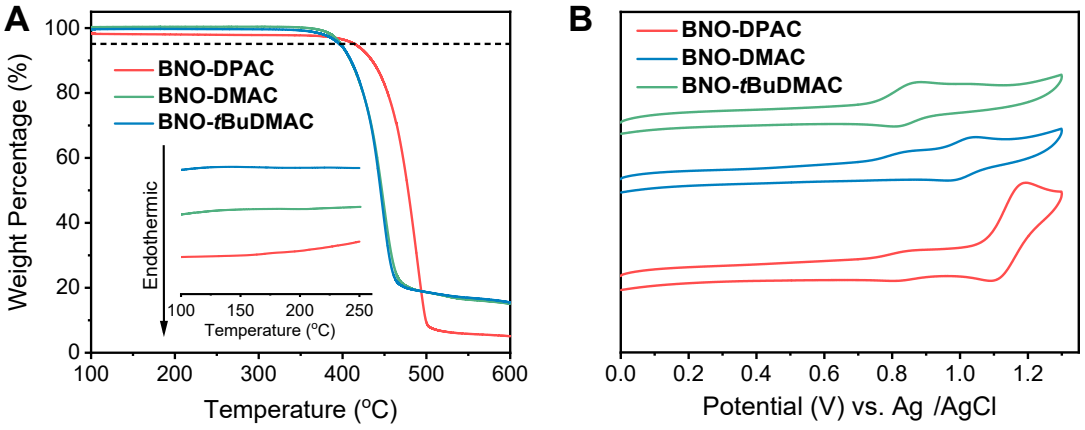
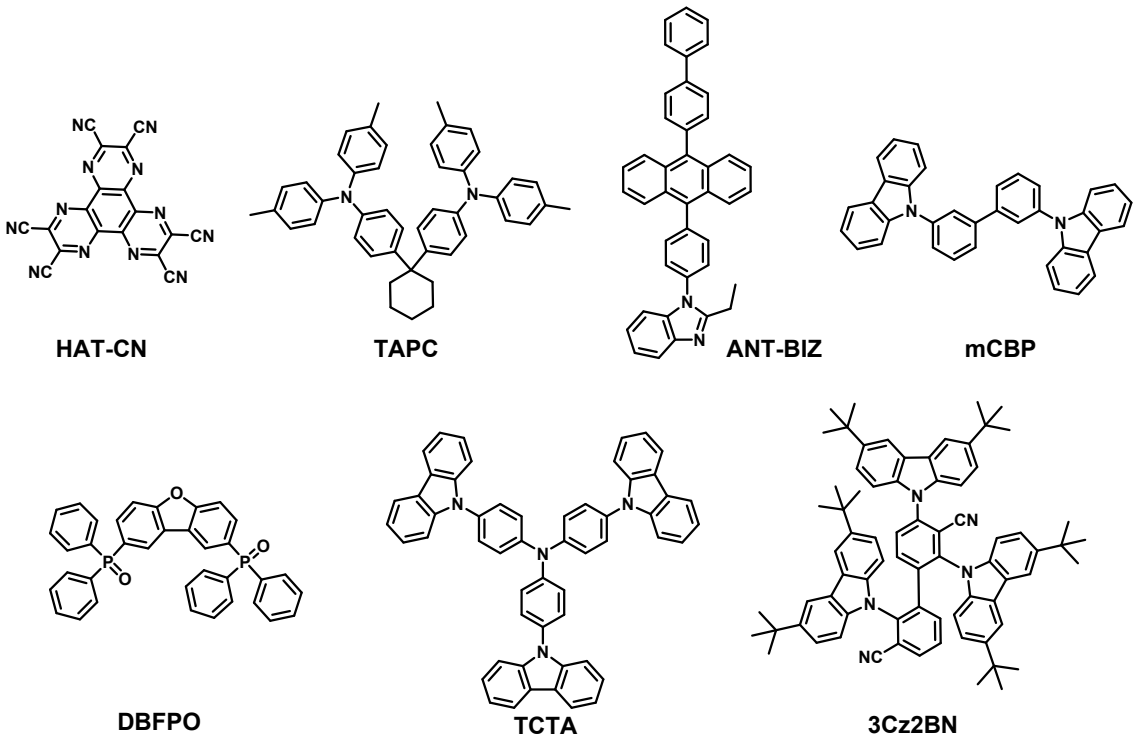


Fig. S15. (A) Thermal gravimetric analysis (TGA) curves at a heating rate of 10 °C min^{-1}, inset: differential scanning calorimetry (DSC) traces at a heating rate of 10 °C min^{-1}; (B) the oxidation curves obtained from the cyclic voltammetry (CV) measurement for **BNO-DPAC**, **BNO-DMAC** and **BNO-*t*BuDMAC**.



Scheme S2. Chemical structures of materials utilized in device fabrication.

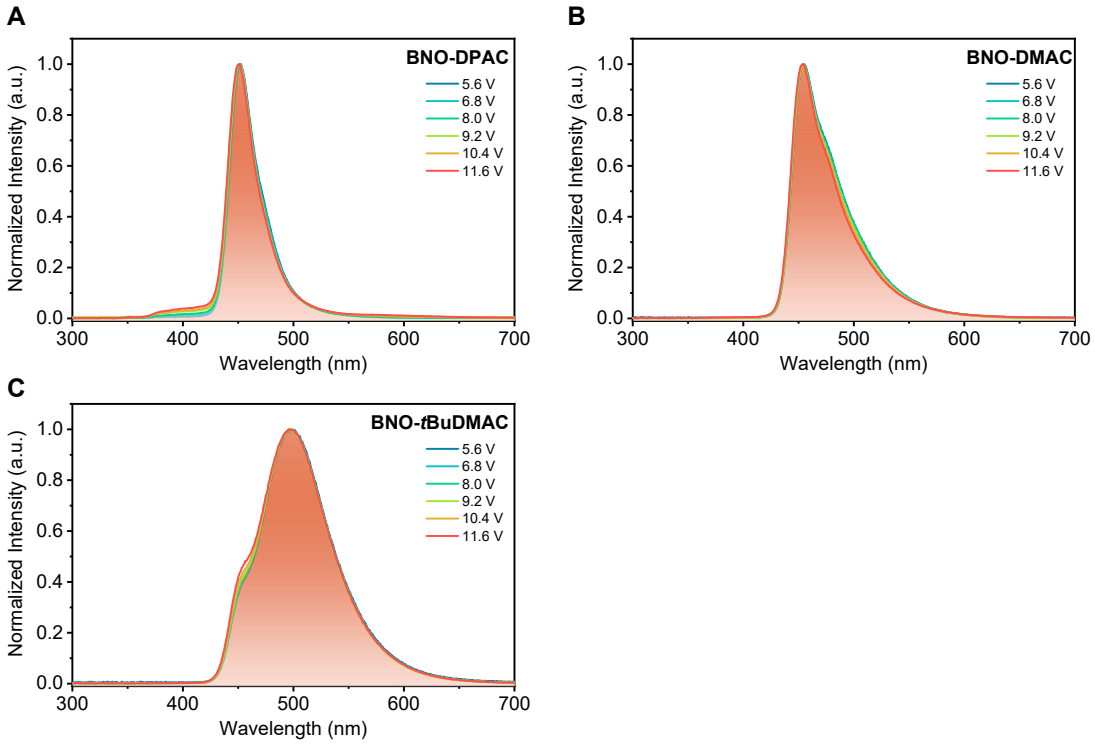


Fig. S16. Normalized electroluminescence (EL) spectra of the sensitizer-free devices based on (A) **BNO-DPAC**, (B) **BNO-DMAC** and (C) **BNO-*t*BuDMAC**.

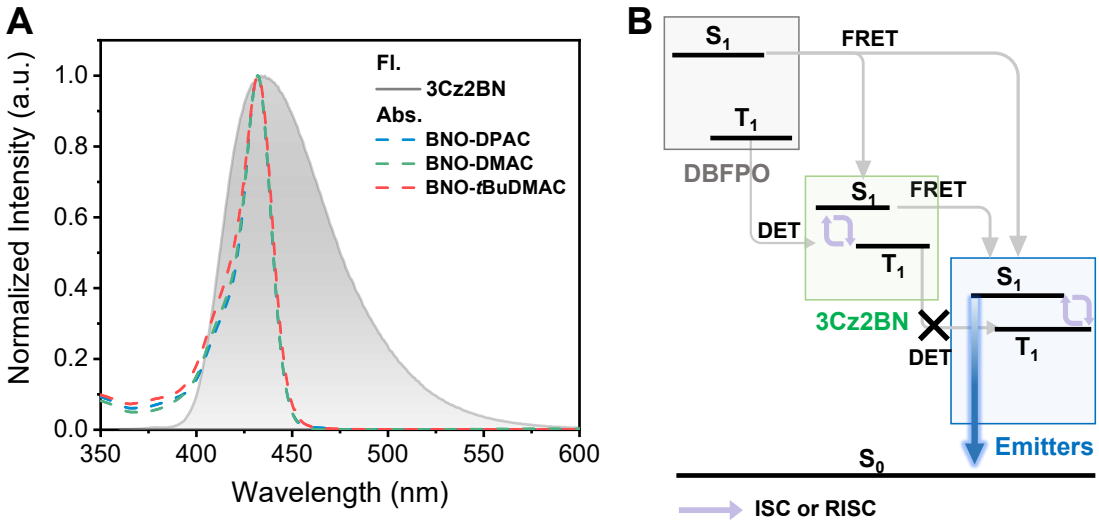


Fig. S17. (A) Comparison between fluorescence spectra (Fl., measured at 300 K) of the sensitizer (3Cz2BN) and UV-vis absorption spectrum (Abs., measured at 300 K) of the emitters in toluene solution; (B) diagram of energy transfer mechanism in the hyperfluorescent (HF) devices.

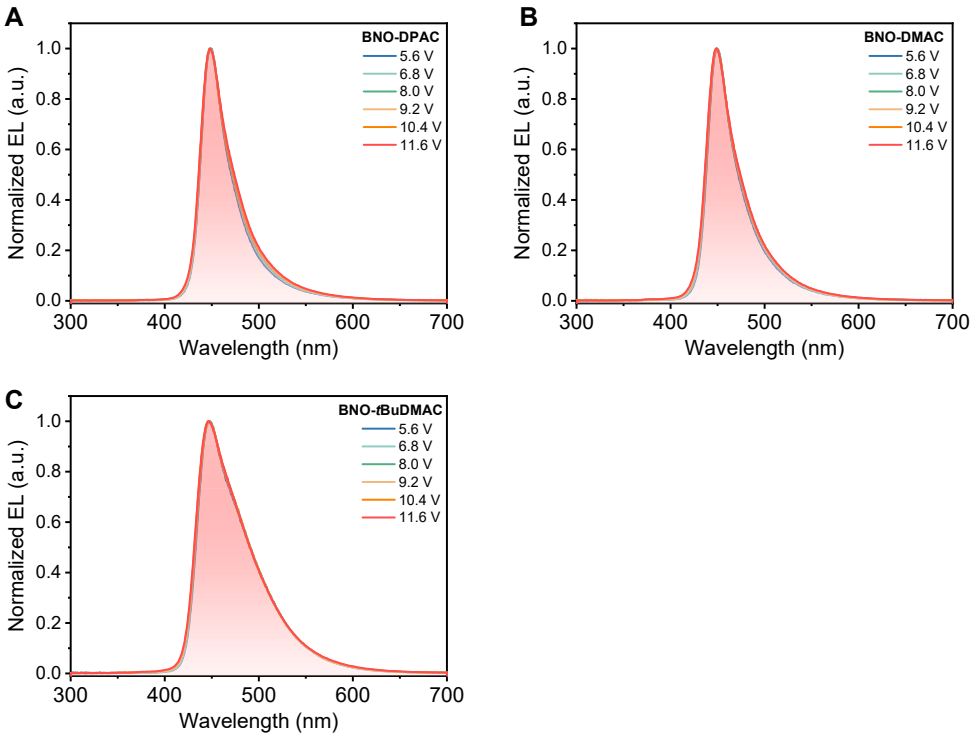


Fig. S18. Normalized EL spectra of the sensitizer-assisted devices based on (A) **BNO-DPAC**, (B) **BNO-DMAC** and (C) **BNO-*t*BuDMAC**.

Table S1. Crystal data and structure refinement for **BNO-DPAC**.

Identification code	**BNO-DPAC**
Empirical formula	$C_{61}H_{55}BN_2O$
Formula weight	842.88
Temperature/K	296.15
Crystal system	monoclinic
Space group	P21/n
a/Å	11.6117(3)
b/Å	28.5813(8)
c/Å	14.5834(4)
α/°	90
β/°	93.2900(10)
γ/°	90
Volume/Å^3	4831.9(2)
Z	4
ρ_{calc}g/cm^3	1.159
μ/mm^{-1}	0.067
F(000)	1792.0
Crystal size/mm^3	0.2 × 0.15 × 0.12
Radiation	MoKα (λ = 0.71073)
2Θ range for data collection/°	4.364 to 54.254
Index ranges	-14 ≤ h ≤ 14, -36 ≤ k ≤ 36, -18 ≤ l ≤ 18
Reflections collected	72191
Independent reflections	10665 [R_{int} = 0.0661, R_{sigma} = 0.0389]
Data/restraints/parameters	10665/120/635
Goodness-of-fit on F^2	1.016
Final R indexes [I>=2σ (I)]	R^1 = 0.0592, wR^2 = 0.1474
Final R indexes [all data]	R^1 = 0.1039, wR^2 = 0.1804
Largest diff. peak/hole / e Å^{-3}	0.31/-0.19

Table S2. Crystal data and structure refinement for **BNO-*t*BuDMAC**.

Identification code	**BNO-*t*BuDMAC**
Empirical formula	$C_{59}H_{67}BN_2O$
Formula weight	830.95
Temperature/K	170.00
Crystal system	monoclinic
Space group	P21/c
a/Å	25.778(4)
b/Å	5.9420(9)
c/Å	34.417(5)
α/°	90
β/°	109.434(5)
γ/°	90
Volume/Å^3	4971.4(13)
Z	4
ρcalcg/cm^3	1.110
μ/mm^{-1}	0.310
F(000)	1792.0
Crystal size/mm^3	0.4 × 0.02 × 0.02
Radiation	GaKα (λ = 1.34139)
2Θ range for data collection/°	4.74 to 114.322
Index ranges	$-30 \leq h \leq 32$, $-7 \leq k \leq 7$, $-42 \leq l \leq 43$
Reflections collected	59752
Independent reflections	10203 [R_{int} = 0.1721, R_{sigma} = 0.1817]
Data/restraints/parameters	10203/0/585
Goodness-of-fit on F^2	1.032
Final R indexes [I>=2σ(I)]	R_1 = 0.0945, wR_2 = 0.2254
Final R indexes [all data]	R_1 = 0.1735, wR_2 = 0.2673
Largest diff. peak/hole / e Å^{-3}	0.36/-0.28

Table S3. Cartesian coordinates of **BNO** at the optimized S_0 geometry.

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-5.395603	-1.141965	0.559679
2	6	0	-4.839941	-2.182357	-0.080363
3	6	0	-3.600770	-2.106607	-0.593540
4	6	0	-2.957002	-0.935814	-0.442226
5	6	0	-3.504359	0.099092	0.211129
6	6	0	-4.746590	0.026856	0.725205
7	8	0	-3.009955	-3.158809	-1.246358
8	6	0	-1.694897	-3.383105	-0.917707
9	6	0	-0.809488	-2.373694	-0.794466
10	5	0	-1.490666	-0.963104	-1.061220
11	6	0	0.495858	-2.467838	-0.445662
12	7	0	1.238559	-1.417376	-0.322673
13	6	0	0.792452	-0.228214	-0.524786
14	6	0	-0.425922	0.197626	-0.877086
15	6	0	1.713247	0.724350	-0.352744
16	6	0	1.473352	2.032320	-0.515575
17	6	0	0.249034	2.451478	-0.892093
18	6	0	-0.684544	1.497515	-1.082587
19	6	0	-1.233873	-4.624843	-0.709442
20	6	0	0.051056	-4.801836	-0.384557
21	6	0	0.874655	-3.749467	-0.255739
22	6	0	2.480013	-1.253730	-0.005041
23	6	0	2.811633	0.052106	-0.011593
24	6	0	3.501701	-2.065450	0.325353
25	6	0	4.728800	-1.595432	0.614826
26	6	0	5.033322	-0.285007	0.598192
27	6	0	4.024856	0.542687	0.272920
28	6	0	-5.409181	1.189140	1.474983
29	6	0	-4.550621	2.474284	1.524637
30	6	0	-6.739162	1.560450	0.781373
31	6	0	-5.685069	0.759210	2.932186
32	6	0	-0.098529	3.927818	-1.116647
33	6	0	1.059378	4.899108	-0.792323
34	6	0	-0.481124	4.140304	-2.597555
35	6	0	-1.288987	4.318458	-0.211798
36	6	0	6.425439	0.268169	0.922961
37	6	0	7.468162	-0.819995	1.266286
38	6	0	6.962892	1.049358	-0.296791
39	6	0	6.327519	1.212409	2.141504
40	1	0	-6.412978	-1.275884	0.960797

41	1	0	-5.407523	-3.122406	-0.185534
42	1	0	-2.903118	1.008089	0.327331
43	1	0	2.293847	2.742295	-0.348245
44	1	0	-1.692601	1.770822	-1.427280
45	1	0	-1.909184	-5.490926	-0.803218
46	1	0	0.425266	-5.826314	-0.213026
47	1	0	1.885943	-4.046417	0.023302
48	1	0	3.426848	-3.154360	0.386729
49	1	0	5.498635	-2.339405	0.872997
50	1	0	4.192158	1.628825	0.237720
51	1	0	-5.076365	3.292025	2.067562
52	1	0	-3.588195	2.316533	2.061890
53	1	0	-4.334090	2.864195	0.504355
54	1	0	-7.229690	2.426311	1.280921
55	1	0	-7.480705	0.731925	0.796348
56	1	0	-6.567719	1.839588	-0.283268
57	1	0	-4.740736	0.469267	3.446769
58	1	0	-6.147893	1.585293	3.518174
59	1	0	-6.381899	-0.105439	2.997578
60	1	0	0.756088	5.958298	-0.954109
61	1	0	1.378125	4.822010	0.271976
62	1	0	1.943861	4.727379	-1.446531
63	1	0	-0.718484	5.208200	-2.805478
64	1	0	-1.376912	3.552659	-2.896737
65	1	0	0.355182	3.843574	-3.270967
66	1	0	-1.054507	4.128893	0.860611
67	1	0	-1.541703	5.397833	-0.315542
68	1	0	-2.217537	3.758046	-0.456058
69	1	0	8.461789	-0.370922	1.492330
70	1	0	7.177701	-1.404184	2.168749
71	1	0	7.628910	-1.523312	0.418093
72	1	0	7.987526	1.442200	-0.107678
73	1	0	6.332864	1.928396	-0.556489
74	1	0	7.014139	0.395146	-1.196921
75	1	0	5.676383	2.093777	1.950790
76	1	0	5.916731	0.676957	3.027667
77	1	0	7.326668	1.614365	2.424590

Table S4. Cartesian coordinates of **BNO** at the optimized S_1 geometry.

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-5.756868	-1.450088	0.198088

2	6	0	-4.941212	-2.543925	-0.018968
3	6	0	-3.554279	-2.359782	-0.112573
4	6	0	-2.976376	-1.086667	-0.008476
5	6	0	-3.853665	-0.004869	0.234487
6	6	0	-5.230810	-0.147255	0.339295
7	8	0	-2.835284	-3.494703	-0.311890
8	6	0	-1.482565	-3.520471	-0.340557
9	6	0	-0.716411	-2.347935	-0.220279
10	5	0	-1.438076	-0.994152	-0.148491
11	6	0	0.702025	-2.476373	-0.252808
12	7	0	1.451907	-1.307214	-0.100478
13	6	0	0.864935	-0.047372	-0.181111
14	6	0	-0.506807	0.239859	-0.246483
15	6	0	1.857176	0.948159	-0.174547
16	6	0	1.486444	2.286303	-0.284523
17	6	0	0.131498	2.631114	-0.399540
18	6	0	-0.824859	1.602690	-0.374418
19	6	0	-0.903732	-4.779349	-0.517265
20	6	0	0.478971	-4.855823	-0.597088
21	6	0	1.289975	-3.725987	-0.472606
22	6	0	2.842037	-1.126250	0.045487
23	6	0	3.128044	0.260152	-0.025025
24	6	0	3.877455	-2.024000	0.307916
25	6	0	5.176902	-1.529110	0.430035
26	6	0	5.489683	-0.165283	0.313735
27	6	0	4.433666	0.726376	0.097186
28	6	0	-6.176603	1.028457	0.598675
29	6	0	-5.419970	2.355251	0.711706
30	6	0	-7.179109	1.138658	-0.561768
31	6	0	-6.937885	0.789054	1.912776
32	6	0	-0.340245	4.083851	-0.542170
33	6	0	0.832199	5.068718	-0.535158
34	6	0	-1.100476	4.244655	-1.868857
35	6	0	-1.274262	4.435418	0.627757
36	6	0	6.920514	0.370945	0.436464
37	6	0	7.936433	-0.750611	0.670655
38	6	0	7.299164	1.104027	-0.860780
39	6	0	6.998726	1.350083	1.619196
40	1	0	-6.834861	-1.610471	0.270541
41	1	0	-5.344753	-3.551995	-0.114696
42	1	0	-3.411398	0.980305	0.364913
43	1	0	2.259934	3.054435	-0.284577
44	1	0	-1.874957	1.880687	-0.473246
45	1	0	-1.544091	-5.655354	-0.608679
46	1	0	0.951513	-5.823975	-0.770814

47	1	0	2.361472	-3.829546	-0.598524
48	1	0	3.708540	-3.085353	0.460851
49	1	0	5.967730	-2.249542	0.634756
50	1	0	4.619894	1.800976	0.034521
51	1	0	-6.133292	3.172974	0.890130
52	1	0	-4.705689	2.343955	1.548422
53	1	0	-4.868810	2.586105	-0.212696
54	1	0	-7.870046	1.978195	-0.389691
55	1	0	-7.780831	0.224327	-0.665983
56	1	0	-6.655071	1.309916	-1.513584
57	1	0	-6.238514	0.706914	2.757715
58	1	0	-7.626931	1.624142	2.112136
59	1	0	-7.531980	-0.135380	1.873321
60	1	0	0.452547	6.095556	-0.639100
61	1	0	1.400053	5.014481	0.405467
62	1	0	1.523230	4.880386	-1.370085
63	1	0	-1.444992	5.283575	-1.987108
64	1	0	-1.982847	3.589817	-1.911223
65	1	0	-0.452525	3.994578	-2.721784
66	1	0	-0.752974	4.322074	1.589722
67	1	0	-1.619263	5.477221	0.540209
68	1	0	-2.162731	3.787370	0.645789
69	1	0	8.947088	-0.322852	0.741603
70	1	0	7.734540	-1.290874	1.607301
71	1	0	7.935301	-1.475915	-0.156352
72	1	0	8.324601	1.498409	-0.790467
73	1	0	6.625125	1.949817	-1.058671
74	1	0	7.248048	0.421933	-1.722180
75	1	0	6.320920	2.204851	1.482668
76	1	0	6.725245	0.847734	2.558709
77	1	0	8.021818	1.743695	1.720855

Table S5. Cartesian coordinates of **BNO-DPAC** at the optimized S_0 geometry.

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	5.323194	2.229834	0.382811
2	6	0	3.948958	2.301320	0.179181
3	6	0	3.203265	1.102466	0.099650
4	6	0	3.783019	-0.171966	0.174302
5	6	0	5.180228	-0.183362	0.396117
6	6	0	5.960641	0.976149	0.505513
7	7	0	1.849113	1.398665	-0.075064

8	6	0	0.874692	0.398435	-0.055938
9	6	0	1.324911	-0.957848	-0.078514
10	5	0	2.806363	-1.352746	-0.016758
11	6	0	0.343083	-1.970938	-0.094241
12	8	0	0.674982	-3.285555	-0.121421
13	6	0	1.963664	-3.731364	-0.177003
14	6	0	3.079953	-2.868588	-0.141018
15	6	0	-0.493903	0.684231	0.021967
16	6	0	-1.424575	-0.360924	0.000987
17	6	0	-1.027246	-1.692789	-0.072019
18	6	0	2.113193	-5.119250	-0.269911
19	6	0	3.387929	-5.669945	-0.343284
20	6	0	4.540725	-4.859255	-0.334974
21	6	0	4.348068	-3.479927	-0.236659
22	6	0	3.176286	4.775602	-0.068999
23	6	0	2.087008	5.613858	-0.330730
24	6	0	0.832047	5.006305	-0.546749
25	6	0	0.629255	3.626867	-0.484607
26	6	0	1.721805	2.805593	-0.184618
27	6	0	3.004086	3.389894	-0.005643
28	6	0	7.478677	0.924174	0.745942
29	6	0	8.003824	-0.517368	0.843925
30	6	0	8.205311	1.622641	-0.422740
31	6	0	7.810745	1.649678	2.066887
32	6	0	5.966209	-5.425293	-0.434173
33	6	0	5.975777	-6.960141	-0.499758
34	6	0	6.642133	-4.878669	-1.709438
35	6	0	6.778711	-4.987054	0.802910
36	6	0	2.213438	7.143125	-0.405903
37	6	0	3.651821	7.616007	-0.145659
38	6	0	1.792216	7.624460	-1.810388
39	6	0	1.293960	7.782868	0.655700
40	7	0	-2.820243	-0.069915	0.087360
41	6	0	-3.437701	-0.066789	1.350174
42	6	0	-4.845619	-0.107564	1.418073
43	6	0	-5.597855	-0.395685	0.116226
44	6	0	-4.928007	0.415813	-0.998378
45	6	0	-3.515881	0.436126	-1.023691
46	6	0	-2.680870	-0.011352	2.533065
47	6	0	-3.320255	0.031221	3.771184
48	6	0	-4.714913	0.031152	3.846397
49	6	0	-5.464482	-0.040874	2.669522
50	6	0	-5.632535	0.980991	-2.064891
51	6	0	-4.969710	1.524074	-3.168455
52	6	0	-3.574905	1.486907	-3.212178

53	6	0	-2.848552	0.950702	-2.149152
54	6	0	-7.082439	-0.033252	0.251001
55	6	0	-8.109124	-0.971795	0.106616
56	6	0	-9.450594	-0.593742	0.246587
57	6	0	-9.784208	0.729228	0.533140
58	6	0	-8.764456	1.677145	0.680711
59	6	0	-7.431221	1.297523	0.541427
60	6	0	-5.412635	-1.901665	-0.222865
61	6	0	-5.240872	-2.855746	0.790052
62	6	0	-5.100842	-4.212133	0.483323
63	6	0	-5.128713	-4.641271	-0.845474
64	6	0	-5.301662	-3.699512	-1.862922
65	6	0	-5.439307	-2.344519	-1.553405
66	1	0	5.903876	3.152177	0.450207
67	1	0	5.669766	-1.147445	0.495918
68	1	0	-0.865781	1.694624	0.140173
69	1	0	-1.763041	-2.496276	-0.089456
70	1	0	1.220387	-5.746570	-0.287726
71	1	0	3.477018	-6.753666	-0.415802
72	1	0	5.222863	-2.832370	-0.247230
73	1	0	4.175312	5.184560	0.077754
74	1	0	-0.031573	5.631000	-0.782083
75	1	0	-0.359944	3.235060	-0.703145
76	1	0	9.091184	-0.505483	1.014843
77	1	0	7.542591	-1.065902	1.679562
78	1	0	7.819973	-1.084271	-0.081821
79	1	0	9.296346	1.597587	-0.268886
80	1	0	7.906355	2.677206	-0.518811
81	1	0	7.981260	1.122089	-1.377652
82	1	0	7.496804	2.704082	2.043473
83	1	0	7.302544	1.167209	2.916292
84	1	0	8.896029	1.627739	2.257695
85	1	0	7.012795	-7.324214	-0.563308
86	1	0	5.519808	-7.409889	0.395866
87	1	0	5.438292	-7.335017	-1.384451
88	1	0	7.667961	-5.271140	-1.801212
89	1	0	6.703031	-3.779953	-1.697267
90	1	0	6.079430	-5.173224	-2.608952
91	1	0	6.312112	-5.355334	1.729839
92	1	0	7.804386	-5.387034	0.751585
93	1	0	6.851449	-3.891505	0.876144
94	1	0	3.698676	8.714423	-0.201897
95	1	0	4.004459	7.319008	0.854028
96	1	0	4.355049	7.215430	-0.891948
97	1	0	1.877287	8.720888	-1.883054

98	1	0	0.750766	7.354255	-2.039978
99	1	0	2.433900	7.177896	-2.585911
100	1	0	1.576073	7.453179	1.667789
101	1	0	1.369246	8.881802	0.618539
102	1	0	0.238948	7.513995	0.497398
103	1	0	-1.592849	0.007729	2.479235
104	1	0	-2.718846	0.075888	4.682338
105	1	0	-5.218739	0.070183	4.814421
106	1	0	-6.552853	-0.079350	2.723348
107	1	0	-6.722626	0.962702	-2.045435
108	1	0	-5.541170	1.950577	-3.995433
109	1	0	-3.038918	1.884851	-4.077262
110	1	0	-1.760650	0.933857	-2.191179
111	1	0	-7.865755	-2.010319	-0.116811
112	1	0	-10.235788	-1.344710	0.129549
113	1	0	-10.830674	1.024079	0.642063
114	1	0	-9.011219	2.717605	0.906239
115	1	0	-6.640037	2.040696	0.659156
116	1	0	-5.210744	-2.538072	1.832341
117	1	0	-4.964127	-4.935492	1.291069
118	1	0	-5.013109	-5.700682	-1.086780
119	1	0	-5.322738	-4.018369	-2.908014
120	1	0	-5.563047	-1.622001	-2.360349

Table S6. Cartesian coordinates of **BNO-DPAC** at the optimized S_1 geometry.

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	5.228223	2.340421	0.475796
2	6	0	3.865073	2.356901	0.215023
3	6	0	3.172491	1.133544	0.111827
4	6	0	3.799570	-0.113567	0.210615
5	6	0	5.181112	-0.071993	0.493676
6	6	0	5.907048	1.116389	0.632926
7	7	0	1.820756	1.374649	-0.112260
8	6	0	0.882139	0.344256	-0.096775
9	6	0	1.378427	-0.990808	-0.120699
10	5	0	2.874707	-1.330719	-0.031074
11	6	0	0.440072	-2.037049	-0.145441
12	8	0	0.817940	-3.333219	-0.173193
13	6	0	2.117824	-3.730644	-0.231228
14	6	0	3.202044	-2.837052	-0.179751
15	6	0	-0.491529	0.583157	-0.013280

16	6	0	-1.381166	-0.495785	-0.043624
17	6	0	-0.939025	-1.808327	-0.128345
18	6	0	2.312848	-5.109789	-0.343777
19	6	0	3.601759	-5.614857	-0.425176
20	6	0	4.725119	-4.767917	-0.407605
21	6	0	4.488436	-3.400311	-0.287820
22	6	0	3.004571	4.794035	-0.095259
23	6	0	1.897439	5.576895	-0.421578
24	6	0	0.683718	4.914523	-0.691867
25	6	0	0.534475	3.533608	-0.617031
26	6	0	1.644209	2.767636	-0.243984
27	6	0	2.884650	3.404854	-0.018481
28	6	0	7.409478	1.131744	0.941028
29	6	0	7.986953	-0.281777	1.064278
30	6	0	8.154566	1.859372	-0.190064
31	6	0	7.648082	1.868854	2.269055
32	6	0	6.163503	-5.285848	-0.516979
33	6	0	6.214134	-6.812978	-0.618241
34	6	0	6.823429	-4.692383	-1.772333
35	6	0	6.955969	-4.855063	0.728288
36	6	0	1.958867	7.104740	-0.517120
37	6	0	3.355823	7.639427	-0.190332
38	6	0	1.593339	7.543143	-1.944684
39	6	0	0.959954	7.715626	0.479173
40	7	0	-2.784426	-0.253732	0.055660
41	6	0	-3.371156	-0.234322	1.332258
42	6	0	-4.774649	-0.216506	1.432984
43	6	0	-5.567822	-0.457150	0.149334
44	6	0	-4.891594	0.335483	-0.970251
45	6	0	-3.483979	0.294874	-1.030242
46	6	0	-2.588155	-0.220475	2.496290
47	6	0	-3.196816	-0.158939	3.745805
48	6	0	-4.584192	-0.098430	3.853552
49	6	0	-5.360839	-0.129686	2.696396
50	6	0	-5.596439	0.943779	-2.009394
51	6	0	-4.940202	1.466640	-3.122759
52	6	0	-3.554150	1.363653	-3.204493
53	6	0	-2.825718	0.785706	-2.168687
54	6	0	-7.029002	-0.026468	0.320429
55	6	0	-8.104856	-0.902357	0.170287
56	6	0	-9.419032	-0.452633	0.338215
57	6	0	-9.673574	0.876023	0.657714
58	6	0	-8.603076	1.761644	0.810557
59	6	0	-7.298384	1.313153	0.643589
60	6	0	-5.469360	-1.963821	-0.203626

61	6	0	-5.389646	-2.933524	0.803163
62	6	0	-5.362269	-4.291966	0.488038
63	6	0	-5.409575	-4.707630	-0.841229
64	6	0	-5.484193	-3.750827	-1.851623
65	6	0	-5.511256	-2.392905	-1.535617
66	1	0	5.770360	3.284963	0.563312
67	1	0	5.702663	-1.017593	0.623736
68	1	0	-0.899527	1.579312	0.123369
69	1	0	-1.645567	-2.637362	-0.151593
70	1	0	1.440281	-5.762548	-0.370943
71	1	0	3.727769	-6.693723	-0.513285
72	1	0	5.341788	-2.721302	-0.296293
73	1	0	3.978020	5.247522	0.090634
74	1	0	-0.189493	5.500498	-0.984913
75	1	0	-0.422030	3.094822	-0.886879
76	1	0	9.063124	-0.221420	1.282095
77	1	0	7.510555	-0.845086	1.880376
78	1	0	7.865483	-0.851864	0.130694
79	1	0	9.235604	1.878575	0.016850
80	1	0	7.815081	2.899610	-0.297049
81	1	0	7.994414	1.350254	-1.151853
82	1	0	7.289659	2.907452	2.225403
83	1	0	7.123353	1.364061	3.093437
84	1	0	8.723165	1.892958	2.504685
85	1	0	7.260577	-7.143625	-0.688814
86	1	0	5.769453	-7.292044	0.266696
87	1	0	5.686637	-7.176947	-1.512353
88	1	0	7.858521	-5.055234	-1.866331
89	1	0	6.852885	-3.593810	-1.731700
90	1	0	6.270434	-4.982630	-2.677742
91	1	0	6.498925	-5.263096	1.641797
92	1	0	7.992550	-5.220344	0.665536
93	1	0	6.990260	-3.760042	0.826879
94	1	0	3.356547	8.736885	-0.260046
95	1	0	3.663726	7.367018	0.829982
96	1	0	4.109721	7.258306	-0.894898
97	1	0	1.636502	8.639964	-2.028188
98	1	0	0.577748	7.224623	-2.219629
99	1	0	2.293550	7.111883	-2.675172
100	1	0	1.203625	7.414247	1.508576
101	1	0	0.990267	8.814610	0.422810
102	1	0	-0.070156	7.395245	0.267479
103	1	0	-1.501823	-0.249879	2.421665
104	1	0	-2.573851	-0.147588	4.641405
105	1	0	-5.062851	-0.042868	4.831555

106	1	0	-6.448811	-0.118577	2.775079
107	1	0	-6.685782	0.974641	-1.961591
108	1	0	-5.511983	1.927233	-3.928685
109	1	0	-3.024146	1.740798	-4.080486
110	1	0	-1.742054	0.714828	-2.246237
111	1	0	-7.925663	-1.948101	-0.080303
112	1	0	-10.245323	-1.154690	0.216117
113	1	0	-10.698980	1.225041	0.788278
114	1	0	-8.788459	2.807287	1.061485
115	1	0	-6.463648	2.007790	0.763955
116	1	0	-5.345749	-2.627438	1.849197
117	1	0	-5.298658	-5.028530	1.290678
118	1	0	-5.383492	-5.770006	-1.088341
119	1	0	-5.516185	-4.059767	-2.897690
120	1	0	-5.562523	-1.659152	-2.341039

Table S7. Cartesian coordinates of **BNO-DMAC** at the optimized S_0 geometry.

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-3.750349	2.169565	-0.788121
2	6	0	-2.431831	2.057100	-0.581770
3	6	0	-1.768710	0.899977	-0.655934
4	6	0	-2.507175	-0.177038	-0.947850
5	6	0	-3.823609	-0.088258	-1.190715
6	6	0	-4.484150	1.083328	-1.103851
7	7	0	-0.507700	1.016859	-0.432774
8	6	0	0.299597	0.008616	-0.473956
9	6	0	-0.149401	-1.238419	-0.725566
10	5	0	-1.684940	-1.532160	-1.005780
11	6	0	0.593182	-2.357859	-0.746762
12	8	0	0.025156	-3.595622	-0.936357
13	6	0	-1.157163	-3.804498	-0.270160
14	6	0	-2.113551	-2.859542	-0.239562
15	6	0	1.639860	0.035213	-0.319156
16	6	0	2.495175	-1.014758	-0.336596
17	6	0	1.911346	-2.211922	-0.548723
18	6	0	-1.428699	-4.951240	0.375256
19	6	0	-2.587909	-5.134101	1.027813
20	6	0	-3.536668	-4.179277	1.075096
21	6	0	-3.264346	-3.032568	0.424144
22	6	0	-1.640302	4.265307	-0.067175
23	6	0	-0.579398	5.020176	0.266695

24	6	0	0.588556	4.362725	0.388403
25	6	0	0.713865	3.040051	0.180773
26	6	0	-0.331838	2.270969	-0.177086
27	6	0	-1.492750	2.949082	-0.269122
28	6	0	-5.991942	1.209147	-1.352403
29	6	0	-6.686953	-0.132734	-1.679554
30	6	0	-6.672070	1.775611	-0.086078
31	6	0	-6.235660	2.160030	-2.544549
32	6	0	-4.865648	-4.344705	1.821928
33	6	0	-5.031171	-5.721220	2.504825
34	6	0	-4.969968	-3.267493	2.924607
35	6	0	-6.036543	-4.180352	0.827088
36	6	0	-0.664219	6.529226	0.521356
37	6	0	-2.079209	7.117900	0.318127
38	6	0	-0.247491	6.825259	1.978838
39	6	0	0.282637	7.267619	-0.450518
40	7	0	3.773226	-0.888670	-0.158323
41	6	0	4.588492	-1.548171	-0.922474
42	6	0	5.935580	-1.498637	-0.790414
43	6	0	6.596163	-0.606881	0.237561
44	6	0	5.521247	0.110859	1.023382
45	6	0	4.206280	-0.105955	0.782161
46	6	0	4.188864	-2.232922	-2.025792
47	6	0	4.989348	-2.939245	-2.837201
48	6	0	6.302401	-2.958629	-2.604232
49	6	0	6.753810	-2.208637	-1.594667
50	6	0	5.935476	0.944889	1.999683
51	6	0	5.089838	1.566646	2.826631
52	6	0	3.792811	1.285520	2.695085
53	6	0	3.397179	0.457341	1.717623
54	6	0	7.477299	0.436009	-0.489399
55	6	0	7.433012	-1.477107	1.204502
56	1	0	-4.225707	3.157376	-0.704927
57	1	0	-4.341116	-1.014974	-1.472927
58	1	0	2.129451	1.007177	-0.260121
59	1	0	2.492402	-3.150132	-0.501523
60	1	0	-0.675505	-5.757435	0.369560
61	1	0	-2.726478	-6.101925	1.532544
62	1	0	-3.990676	-2.209628	0.440935
63	1	0	-2.639540	4.707929	-0.173160
64	1	0	1.493583	4.919992	0.682752
65	1	0	1.728096	2.668036	0.353518
66	1	0	-7.780033	0.006648	-1.840378
67	1	0	-6.291953	-0.589727	-2.615014
68	1	0	-6.583932	-0.867174	-0.848646

69	1	0	-7.775188	1.851931	-0.217448
70	1	0	-6.316448	2.796782	0.174037
71	1	0	-6.482734	1.119303	0.794015
72	1	0	-5.731643	1.782646	-3.463471
73	1	0	-7.321671	2.255737	-2.771325
74	1	0	-5.860588	3.189894	-2.355119
75	1	0	-6.010035	-5.796951	3.030392
76	1	0	-5.006217	-6.555710	1.767968
77	1	0	-4.248464	-5.899076	3.276699
78	1	0	-5.910937	-3.376364	3.509846
79	1	0	-4.972081	-2.232653	2.516879
80	1	0	-4.118606	-3.345225	3.638660
81	1	0	-5.966864	-4.927735	0.003970
82	1	0	-7.019423	-4.324634	1.330080
83	1	0	-6.068739	-3.170961	0.361144
84	1	0	-2.091162	8.215708	0.504934
85	1	0	-2.442835	6.973232	-0.724366
86	1	0	-2.819670	6.675007	1.022100
87	1	0	-0.324260	7.911842	2.209892
88	1	0	0.803574	6.531095	2.193072
89	1	0	-0.901562	6.281417	2.698018
90	1	0	0.018004	7.045094	-1.509385
91	1	0	0.224191	8.371175	-0.313985
92	1	0	1.349872	6.990118	-0.305794
93	1	0	3.153704	-2.233106	-2.401058
94	1	0	4.583648	-3.475089	-3.712687
95	1	0	6.990188	-3.514510	-3.262180
96	1	0	7.847658	-2.177248	-1.470189
97	1	0	7.006388	1.130561	2.177786
98	1	0	5.450899	2.229269	3.630057
99	1	0	3.067402	1.710035	3.410468
100	1	0	2.319081	0.247397	1.797886
101	1	0	6.862771	1.058386	-1.179918
102	1	0	7.998191	1.127845	0.207201
103	1	0	8.289363	-0.025730	-1.091818
104	1	0	7.945087	-0.882381	1.991579
105	1	0	6.787870	-2.225820	1.719354
106	1	0	8.247625	-2.034995	0.694389

Table S8. Cartesian coordinates of **BNO-DMAC** at the optimized S_1 geometry.

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z

1	6	0	3.376895	3.049268	0.464780
2	6	0	2.055818	2.706640	0.213033
3	6	0	1.709642	1.344562	0.104108
4	6	0	2.644788	0.307288	0.190927
5	6	0	3.968943	0.710343	0.464814
6	6	0	4.356535	2.047291	0.607579
7	7	0	0.339928	1.221402	-0.109183
8	6	0	-0.293474	-0.019870	-0.089279
9	6	0	0.537815	-1.176139	-0.118826
10	5	0	2.071872	-1.109703	-0.047415
11	6	0	-0.090199	-2.433932	-0.134706
12	8	0	0.616566	-3.584302	-0.169982
13	6	0	1.974687	-3.624068	-0.248092
14	6	0	2.784287	-2.475537	-0.207143
15	6	0	-1.682097	-0.154037	0.002556
16	6	0	-2.253673	-1.428723	-0.008110
17	6	0	-1.479437	-2.578042	-0.096938
18	6	0	2.525587	-4.902223	-0.370272
19	6	0	3.900918	-5.048133	-0.472254
20	6	0	4.760324	-3.934205	-0.466068
21	6	0	4.172136	-2.677984	-0.335875
22	6	0	0.580384	4.832502	-0.066791
23	6	0	-0.697068	5.298205	-0.376797
24	6	0	-1.695250	4.341202	-0.646337
25	6	0	-1.473810	2.969381	-0.585441
26	6	0	-0.198620	2.520151	-0.226802
27	6	0	0.831645	3.460285	-0.003622
28	6	0	5.804080	2.457821	0.904729
29	6	0	6.735733	1.246766	1.013605
30	6	0	6.319682	3.362119	-0.226823
31	6	0	5.851276	3.225427	2.236102
32	6	0	6.282599	-4.053331	-0.598901
33	6	0	6.733413	-5.512691	-0.708161
34	6	0	6.742745	-3.305718	-1.861057
35	6	0	6.952299	-3.429336	0.636544
36	6	0	-1.042273	6.788776	-0.455262
37	6	0	0.167879	7.670723	-0.136208
38	6	0	-1.529001	7.127389	-1.873780
39	6	0	-2.154292	7.105195	0.558164
40	7	0	-3.673751	-1.542750	0.085651
41	6	0	-4.260980	-1.699552	1.347148
42	6	0	-5.658534	-1.804502	1.478558
43	6	0	-6.607959	-1.752288	0.282079
44	6	0	-5.844558	-1.544211	-1.025437
45	6	0	-4.440552	-1.454866	-1.081743

46	6	0	-3.449990	-1.746415	2.497361
47	6	0	-4.010335	-1.905045	3.757353
48	6	0	-5.390987	-2.019015	3.901081
49	6	0	-6.188506	-1.965579	2.763168
50	6	0	-6.558654	-1.450258	-2.224621
51	6	0	-5.936133	-1.273734	-3.455672
52	6	0	-4.546510	-1.191317	-3.497638
53	6	0	-3.805632	-1.281888	-2.327050
54	6	0	-7.598854	-0.587096	0.477607
55	6	0	-7.385534	-3.081524	0.201032
56	1	0	3.650899	4.102907	0.556722
57	1	0	4.722320	-0.065018	0.585158
58	1	0	-2.342710	0.696555	0.130231
59	1	0	-1.934590	-3.567340	-0.109486
60	1	0	1.856749	-5.762764	-0.388769
61	1	0	4.306351	-6.055111	-0.567917
62	1	0	4.815074	-1.797181	-0.352802
63	1	0	1.401536	5.525069	0.117100
64	1	0	-2.694497	4.678435	-0.928307
65	1	0	-2.281046	2.295313	-0.856260
66	1	0	7.759602	1.588451	1.223741
67	1	0	6.432580	0.573619	1.829226
68	1	0	6.760742	0.669445	0.076902
69	1	0	7.358963	3.665732	-0.028019
70	1	0	5.716006	4.275904	-0.323898
71	1	0	6.291027	2.833336	-1.190910
72	1	0	5.485843	2.595981	3.060754
73	1	0	6.883896	3.531427	2.464031
74	1	0	5.230945	4.132703	2.202443
75	1	0	7.828783	-5.554878	-0.795893
76	1	0	6.445086	-6.092737	0.181073
77	1	0	6.307001	-6.002654	-1.596010
78	1	0	7.835289	-3.382522	-1.972195
79	1	0	6.481992	-2.238333	-1.815541
80	1	0	6.271915	-3.731013	-2.759533
81	1	0	6.633533	-3.944113	1.554849
82	1	0	8.047418	-3.507972	0.556670
83	1	0	6.697972	-2.364165	0.739706
84	1	0	-0.122171	8.729916	-0.193341
85	1	0	0.549599	7.480783	0.877825
86	1	0	0.986753	7.508362	-0.852526
87	1	0	-1.778397	8.197256	-1.944633
88	1	0	-2.427702	6.554077	-2.142314
89	1	0	-0.749256	6.903076	-2.616445
90	1	0	-1.826705	6.869663	1.581437

91	1	0	-2.416070	8.173576	0.514573
92	1	0	-3.065724	6.525786	0.352756
93	1	0	-2.369370	-1.657189	2.399695
94	1	0	-3.357386	-1.938490	4.630735
95	1	0	-5.842742	-2.145977	4.885020
96	1	0	-7.271075	-2.052769	2.875121
97	1	0	-7.647677	-1.520924	-2.191427
98	1	0	-6.528789	-1.205150	-4.368032
99	1	0	-4.027465	-1.058127	-4.447998
100	1	0	-2.719651	-1.222604	-2.375181
101	1	0	-7.060038	0.368851	0.538580
102	1	0	-8.309450	-0.531090	-0.359184
103	1	0	-8.179250	-0.715923	1.402149
104	1	0	-8.092807	-3.070886	-0.640801
105	1	0	-6.692977	-3.923096	0.059874
106	1	0	-7.958650	-3.256274	1.122976

Table S9. Cartesian coordinates of **BNO-*t*BuDMAC** at the optimized S_0 geometry.

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-4.076056	2.014383	-0.931165
2	6	0	-2.755557	1.956118	-0.715057
3	6	0	-2.055978	0.818274	-0.719907
4	6	0	-2.758500	-0.297036	-0.950624
5	6	0	-4.075972	-0.264283	-1.201808
6	6	0	-4.773699	0.888671	-1.184645
7	7	0	-0.800376	0.988136	-0.500433
8	6	0	0.038590	0.005485	-0.480583
9	6	0	-0.368669	-1.267835	-0.660720
10	5	0	-1.893022	-1.625959	-0.927406
11	6	0	0.409801	-2.361828	-0.615555
12	8	0	-0.116251	-3.626392	-0.736384
13	6	0	-1.296537	-3.837060	-0.067067
14	6	0	-2.283066	-2.923592	-0.092708
15	6	0	1.376642	0.084304	-0.324154
16	6	0	2.265678	-0.936282	-0.277245
17	6	0	1.721563	-2.161788	-0.422004
18	6	0	-1.536161	-4.956544	0.636396
19	6	0	-2.694331	-5.142942	1.289730
20	6	0	-3.673864	-4.218688	1.280091
21	6	0	-3.433096	-3.099143	0.571954
22	6	0	-2.036494	4.214766	-0.328835

23	6	0	-1.001373	5.021204	-0.036987
24	6	0	0.186129	4.409429	0.126894
25	6	0	0.353791	3.081437	-0.002186
26	6	0	-0.665285	2.260045	-0.317742
27	6	0	-1.846539	2.894404	-0.452679
28	6	0	-6.283595	0.951850	-1.443876
29	6	0	-6.935001	-0.428681	-1.689789
30	6	0	-6.986710	1.572856	-0.216165
31	6	0	-6.551596	1.820110	-2.692359
32	6	0	-5.003262	-4.388765	2.025008
33	6	0	-5.130905	-5.733581	2.775863
34	6	0	-5.151378	-3.260957	3.070591
35	6	0	-6.170054	-4.313037	1.014709
36	6	0	-1.134533	6.539249	0.127496
37	6	0	-2.566451	7.069832	-0.113012
38	6	0	-0.732520	6.934482	1.565432
39	6	0	-0.207768	7.248144	-0.884923
40	7	0	3.537870	-0.756990	-0.102800
41	6	0	4.380090	-1.434679	-0.819757
42	6	0	5.723350	-1.331692	-0.687270
43	6	0	6.348065	-0.354347	0.284225
44	6	0	5.244759	0.374074	1.019538
45	6	0	3.940399	0.097179	0.787366
46	6	0	4.015719	-2.201166	-1.879528
47	6	0	4.848151	-2.927922	-2.638885
48	6	0	6.163917	-2.899067	-2.407608
49	6	0	6.567729	-2.063768	-1.442589
50	6	0	5.622658	1.282646	1.942281
51	6	0	4.763415	1.938139	2.732294
52	6	0	3.478719	1.592734	2.607528
53	6	0	3.112325	0.691603	1.684858
54	6	0	7.196648	0.669943	-0.505417
55	6	0	7.208858	-1.131832	1.307643
56	6	0	7.149746	-3.680586	-3.241233
57	6	0	5.237322	2.932650	3.763574
58	1	0	-4.582730	2.989821	-0.907091
59	1	0	-4.562725	-1.221632	-1.431631
60	1	0	1.833652	1.073666	-0.321970
61	1	0	2.331903	-3.076539	-0.318598
62	1	0	-0.757461	-5.737072	0.677861
63	1	0	-2.805785	-6.087185	1.843585
64	1	0	-4.185626	-2.300584	0.540897
65	1	0	-3.048537	4.618657	-0.463651
66	1	0	1.071749	5.011419	0.390484
67	1	0	1.378380	2.752849	0.195415

68	1	0	-8.031395	-0.333840	-1.860661
69	1	0	-6.522774	-0.929081	-2.595045
70	1	0	-6.811898	-1.107538	-0.815462
71	1	0	-8.091037	1.605814	-0.354462
72	1	0	-6.664867	2.618828	-0.018239
73	1	0	-6.780371	0.977837	0.702893
74	1	0	-6.032541	1.403185	-3.585452
75	1	0	-7.639023	1.868287	-2.926954
76	1	0	-6.208887	2.870745	-2.565319
77	1	0	-6.111684	-5.814275	3.297245
78	1	0	-5.072601	-6.603027	2.082450
79	1	0	-4.350088	-5.846712	3.561561
80	1	0	-6.093684	-3.369986	3.653757
81	1	0	-5.182312	-2.248708	2.610484
82	1	0	-4.304330	-3.275471	3.793812
83	1	0	-6.069187	-5.098224	0.231147
84	1	0	-7.152201	-4.463562	1.517356
85	1	0	-6.230664	-3.329957	0.498045
86	1	0	-2.613734	8.175821	0.008448
87	1	0	-2.921468	6.852505	-1.145899
88	1	0	-3.295424	6.646053	0.614404
89	1	0	-0.844371	8.029878	1.731254
90	1	0	0.326534	6.686960	1.798444
91	1	0	-1.371684	6.413673	2.314508
92	1	0	-0.461437	6.954827	-1.929261
93	1	0	-0.301389	8.355434	-0.814467
94	1	0	0.867163	7.013498	-0.722111
95	1	0	2.984084	-2.260889	-2.259746
96	1	0	4.454912	-3.527808	-3.477211
97	1	0	7.657234	-1.982658	-1.307904
98	1	0	6.687273	1.511601	2.102985
99	1	0	2.727098	2.029814	3.286638
100	1	0	2.041641	0.450295	1.777010
101	1	0	6.564390	1.225885	-1.235467
102	1	0	7.690727	1.422039	0.146795
103	1	0	8.026574	0.199186	-1.075580
104	1	0	7.695386	-0.471064	2.057383
105	1	0	6.587068	-1.868450	1.866660
106	1	0	8.045560	-1.692164	0.837325
107	1	0	6.674784	-4.152899	-4.130002
108	1	0	7.964558	-3.019634	-3.614945
109	1	0	7.605901	-4.490828	-2.627941
110	1	0	6.067702	2.507174	4.371739
111	1	0	5.605490	3.855072	3.259317
112	1	0	4.430122	3.230441	4.469565

Table S10. Cartesian coordinates of **BNO-*t*BuDMAC** at the optimized S_1 geometry.

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	3.780716	2.931485	0.519344
2	6	0	2.444584	2.656329	0.264030
3	6	0	2.034983	1.314381	0.127682
4	6	0	2.920795	0.232891	0.189386
5	6	0	4.262655	0.567881	0.468281
6	6	0	4.712547	1.881979	0.638347
7	7	0	0.660944	1.259727	-0.084492
8	6	0	-0.029707	0.048867	-0.091847
9	6	0	0.746721	-1.143772	-0.150067
10	5	0	2.281921	-1.150138	-0.080071
11	6	0	0.060562	-2.370162	-0.194994
12	8	0	0.713405	-3.551232	-0.258375
13	6	0	2.068017	-3.652064	-0.339659
14	6	0	2.929942	-2.543398	-0.273544
15	6	0	-1.422739	-0.022511	-0.000284
16	6	0	-2.054274	-1.268191	-0.042945
17	6	0	-1.333840	-2.449783	-0.160723
18	6	0	2.559830	-4.951026	-0.492245
19	6	0	3.927041	-5.157453	-0.599908
20	6	0	4.836705	-4.084683	-0.569815
21	6	0	4.306804	-2.806182	-0.409802
22	6	0	1.069172	4.853998	0.031607
23	6	0	-0.185994	5.384643	-0.264932
24	6	0	-1.228224	4.480764	-0.550534
25	6	0	-1.070665	3.099209	-0.518783
26	6	0	0.183228	2.584047	-0.173704
27	6	0	1.256544	3.470537	0.066017
28	6	0	6.178380	2.217541	0.940089
29	6	0	7.052723	0.962098	1.017159
30	6	0	6.733109	3.123206	-0.171701
31	6	0	6.264438	2.950546	2.288875
32	6	0	6.351831	-4.270212	-0.708281
33	6	0	6.735591	-5.745869	-0.849827
34	6	0	6.844125	-3.517099	-1.954942
35	6	0	7.050641	-3.704194	0.538939
36	6	0	-0.461968	6.890869	-0.312170
37	6	0	0.788948	7.709251	0.018659
38	6	0	-0.937589	7.280179	-1.721436

39	6	0	-1.554514	7.237876	0.712343
40	7	0	-3.477242	-1.317547	0.046012
41	6	0	-4.077186	-1.502219	1.297975
42	6	0	-5.475937	-1.544792	1.425506
43	6	0	-6.420437	-1.389262	0.233497
44	6	0	-5.643778	-1.154504	-1.062264
45	6	0	-4.239137	-1.134749	-1.113891
46	6	0	-3.279051	-1.637080	2.450094
47	6	0	-3.854383	-1.824286	3.697239
48	6	0	-5.243057	-1.884229	3.851636
49	6	0	-6.016872	-1.738364	2.702158
50	6	0	-6.350967	-0.967980	-2.255634
51	6	0	-5.737682	-0.764058	-3.490434
52	6	0	-4.339691	-0.757924	-3.514220
53	6	0	-3.601782	-0.940031	-2.354477
54	6	0	-7.355524	-0.189287	0.485531
55	6	0	-7.260423	-2.674359	0.087801
56	6	0	-5.867148	-2.108304	5.204157
57	6	0	-6.540335	-0.544924	-4.746134
58	1	0	4.104002	3.968976	0.632561
59	1	0	4.979395	-0.243940	0.570073
60	1	0	-2.042959	0.854471	0.149292
61	1	0	-1.834922	-3.415970	-0.198245
62	1	0	1.852272	-5.779397	-0.529370
63	1	0	4.285749	-6.179533	-0.719219
64	1	0	4.989329	-1.955553	-0.408112
65	1	0	1.921960	5.503987	0.226909
66	1	0	-2.211478	4.869868	-0.821743
67	1	0	-1.909064	2.469011	-0.800504
68	1	0	8.092109	1.250544	1.230930
69	1	0	6.720898	0.284992	1.818205
70	1	0	7.047591	0.406241	0.067237
71	1	0	7.785863	3.373316	0.030753
72	1	0	6.172500	4.066141	-0.245425
73	1	0	6.677729	2.619049	-1.147744
74	1	0	5.871888	2.319623	3.099816
75	1	0	7.310717	3.202760	2.520434
76	1	0	5.686910	3.886181	2.278326
77	1	0	7.827851	-5.836182	-0.940039
78	1	0	6.421444	-6.331308	0.027046
79	1	0	6.286855	-6.196557	-1.747428
80	1	0	7.931999	-3.640624	-2.069821
81	1	0	6.631713	-2.440304	-1.885890
82	1	0	6.353671	-3.901181	-2.861443
83	1	0	6.709806	-4.223760	1.446558

84	1	0	8.140982	-3.830658	0.455119
85	1	0	6.845067	-2.631068	0.665680
86	1	0	0.548477	8.781716	-0.017250
87	1	0	1.164577	7.482404	1.027364
88	1	0	1.597027	7.522386	-0.703915
89	1	0	-1.137202	8.361693	-1.769852
90	1	0	-1.862961	6.754784	-1.997430
91	1	0	-0.171708	7.034925	-2.471881
92	1	0	-1.234229	6.967446	1.729280
93	1	0	-1.767235	8.317783	0.690883
94	1	0	-2.492266	6.704827	0.499857
95	1	0	-2.194485	-1.591730	2.364001
96	1	0	-3.205860	-1.924250	4.570781
97	1	0	-7.104297	-1.776452	2.805644
98	1	0	-7.443258	-0.986953	-2.220676
99	1	0	-3.812988	-0.612478	-4.460320
100	1	0	-2.514250	-0.939295	-2.408679
101	1	0	-6.771726	0.735626	0.593427
102	1	0	-8.060429	-0.058279	-0.347695
103	1	0	-7.943976	-0.335100	1.402407
104	1	0	-7.963787	-2.589509	-0.753117
105	1	0	-6.607958	-3.539956	-0.093516
106	1	0	-7.843739	-2.866050	0.999969
107	1	0	-5.453563	-1.416787	5.952519
108	1	0	-6.954778	-1.961004	5.170116
109	1	0	-5.678442	-3.131163	5.564757
110	1	0	-7.595050	-0.811394	-4.596143
111	1	0	-6.503722	0.508939	-5.062991
112	1	0	-6.151181	-1.149733	-5.577714

Table S11. Summary of TD-DFT data for **BNO, BNO-DPAC**, **BNO-DMAC** and **BNO-*t*BuDMAC** at m062x/def2svp level.

Compound	Transition	Wavelength (nm)	Energy (eV)	Oscillator Strength	Coefficient of Orbital
BNO	S_0-S_1	354	3.51	0.3874	HOMO→LUMO (92.44%)
	S_0-T_1	418	2.97	0.0000	HOMO→LUMO(90.32%)
	S_0-T_2	378	3.28	0.0000	HOMO-1→LUMO (64.77%)
					HOMO-1→LUMO+1(18.52%)
					HOMO→LUMO+1 (3.18%)
	S_0-T_3	341	3.64	0.0000	HOMO-6→LUMO (2.08%)
					HOMO-2→LUMO (64.97%)
					HOMO-2→LUMO+1 (3.08%)
					HOMO→LUMO+1 (5.20%)
					HOMO→LUMO+2 (4.51%)
					HOMO→LUMO+4 (2.16%)
BNO-DPAC	S_0-S_1	354	3.51	0.3748	HOMO-1→LUMO (93.52%)
	S_0-T_1	421	2.95	0.0000	HOMO-1→LUMO(87.84%)
	S_0-T_2	376	3.30	0.0000	HOMO-2→LUMO (64.79%)
					HOMO-2→LUMO+1 (21.21%)
	S_0-T_3	348	3.56	0.0000	HOMO-3→LUMO (59.90%)
					HOMO-3→LUMO+1 (3.63%)
					HOMO-3→LUMO+6 (2.15%)
					HOMO-1→LUMO+1 (7.28%)
					HOMO-1→LUMO+2 (5.11%)
					HOMO→LUMO (2.85%)
BNO-DMAC	S_0-S_1	353	3.51	0.3896	HOMO-1→LUMO (94.73%)
	S_0-T_1	421	2.95	0.0000	HOMO-1→LUMO (89.06%)
	S_0-T_2	376	3.30	0.0000	HOMO-2→LUMO (64.98%)
					HOMO-2→LUMO+1 (21.07%)
	S_0-T_3	351	3.53	0.0000	HOMO-3→LUMO (9.33%)
					HOMO→LUMO (68.13%)
					HOMO→LUMO+1 (4.69%)
					HOMO→LUMO+3 (5.14%)
BNO-*t*BuDMAC	S_0-S_1	365	3.39	0.0054	HOMO→LUMO (84.21%)
					HOMO→LUMO+1 (5.11%)
					HOMO→LUMO+2 (5.80%)
	S_0-T_1	421	2.95	0.0000	HOMO-1→LUMO (89.00%)
	S_0-T_2	376	3.30	0.0000	HOMO-2→LUMO (64.67%)
					HOMO-2→LUMO+1 (20.93%)
	S_0-T_3	367	3.38	0.0000	HOMO→LUMO (84.21%)
					HOMO→LUMO+1 (5.11%)
					HOMO→LUMO+3 (5.81%)

Table S12. The emission profiles of emitters in solution states.

Solvent	**BNO**		**BNO-DPAC**		**BNO-DMAC**		**BNO-*t*BuDMAC**	
	λ_{em} (nm)	FWHM (nm)	λ_{em} (nm)	FWHM (nm)	λ_{em} (nm)	FWHM (nm)	λ_{em} (nm)	FWHM (nm)
Hexane	440	21	440	17	439	17	441	17
Toluene	451	26	447	20	447	21	448/487	81
Dichloromethane	456	31	451	26	451/524	30	447/561	
Acetonitrile	458	35	452/535	33	464/577	115	463/603	

Table S13. Thermal and electrochemical properties of **BNO-DPAC**, **BNO-DMAC** and **BNO-*t*BuDMAC**.

Compounds	T_d (°C)	T_g (°C)	E_{HOMO} (eV)	E_{LUMO} (eV)	E_g (eV)
BNO-DPAC	416	-	-5.28	-2.51	2.77
BNO-DMAC	398	-	-5.18	-2.41	2.77
BNO-*t*BuDMAC	396	-	-5.06	-2.28	2.78

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