Supporting Information

B←N Lewis pair fusion of [6]helicene: one way to integrate circularly polarized luminescence with two-photon absorption

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Materials and Methods

Synthesis and Characterization. All reactions were carried out under nitrogen atmosphere. The starting material **Bpin-HC** and **DiBr-HC** was prepared according to the literature.[1] Melting points (M.p.) were measured on a Tektronix XT-4 instrument. ^{1}H, ^{13}C, ^{11}B and ^{19}F NMR spectra were recorded with a Bruker 400 spectrometer. ^{11}B NMR were acquired with boron-free quartz NMR tubes. To remove the intense background, which was caused by the ^{11}B containing probe, the ^{11}B NMR spectra were processed by subtraction with the signals of a blank sample. Chemical shifts were reported in parts per million (ppm) downfield from $CDCl_3$ (δ = 7.26 ppm) or CD_2Cl_2 (δ = 5.32 ppm) for ^{1}H NMR, relative to the central $CDCl_3$ resonance (δ = 77.16 ppm) or CD_2Cl_2 resonance (δ = 53.84 ppm) for ^{13}C NMR, externally referenced to $BF_3{\cdot}Et_2O$ (δ = 0 ppm) for ^{11}B NMR, and externally referenced to CCl_3F (δ = 0 ppm) for ^{19}F NMR. High-resolution mass spectra (HRMS) were obtained using an electrospray ionization time-of-flight (ESI-TOF) mass spectrometer on a Bruker Apex II mass spectrometer or a Thermo Scientific Orbitrap IQ-X Mass spectrometer.

Absorption and Emission Spectroscopies. UV-vis absorption spectra and fluorescence spectra measurements were performed with a Hitachi U-2910 spectrometer and a Hitachi F-7000 spectrometer, respectively. CD and CPL spectra were measured on Applied Photophysics Chirascan and Jasco CPL 300 spectrometer, respectively.

Fluorescence Quantum Yield Measurements. The absolute fluorescence quantum yields in the solid state were measured using a calibrated integrating sphere (inner diameter: 150 mm) integrated into an Edinburgh Instruments FLSP920 spectrometer. All solid samples were excited at 400 nm with a xenon arc lamp. The instrument response function (IRF) was obtained from the scattering of a blank quartz plate under identical experimental conditions and was subtracted from the measured spectra. The corrected emission spectra were integrated using the F900 software to determine the absolute fluorescence quantum yields.

The Φ_F values in solution were determined by the relative method using coumarin 307 as the as the reference standard (Φ_F = 0.56 in EtOH).[2] A series of dilute solutions (c = 1.0–3.0 × 10^{-5} M) of sample and coumarin 307 were prepared provide a range of absorbance values at the excitation wavelength while remaining in the dilute regime to minimize the inner-filter effects. For each solution, the fluorescence spectra were acquired with the same excitation wavelength (λ_{ex} = 400 nm) and identical instrumental

conditions. The integrated emission intensity (I) was obtained by integrating the entire fluorescence band. At the same time, the absorbance (A) at the excitation wavelength (400 nm) was obtained from the corresponding UV-vis absorption spectrum. For both the sample and coumarin 307, plots of I versus A were constructed and fitted by linear regression. Only datasets displaying excellent linearity ($R^2 > 0.98$) were used. The quantum yield of the sample (Φ_s) was calculated using the Equation (1), which is derived from Equation (2).

$$\Phi_s = \Phi_r \times \frac{slope_s}{slope_r} \times \left(\frac{n_s}{n_r}\right)^2 \quad (1)$$

$$\Phi_s = \Phi_r \times \frac{I_s}{I_r} \times \frac{A_r}{A_s}\left(\frac{n_s}{n_r}\right)^2 \quad (2)$$

where Φ is the fluorescence quantum yield, I is the integrated fluorescence intensity, A is the absorbance value at the excitation wavelength, s*lope* is the slope obtained from the linear fits plot of I versus A, n is the refractive index of the solvent, the subscript r and s mean the reference and experimental sample, respectively.

Fluorescence Lifetime Measurements. Fluorescence lifetimes were recorded using the time-correlated single-photon counting (TCSPC) method using an Edinburgh Instruments FLS920 spectrometer equipped with a high speed photomultiplier tube positioned after a single emission monochromator. Measurements were made in right-angle geometry mode, and the emission was collected through a polarizer set to the magic angle. All samples were excited at 378 nm with Edinburgh picosecond pulsed diode laser EPL-375. The full-width-at-half-maximum (FWHM) of the pulse from the diode laser was 72.5 ps with an instrument response function (IRF) of ca. 200 ps FWHM. The IRF of solution samples were measured from the scatter of an aqueous suspension of Ludox at the excitation wavelength, while the IRF of solid samples were measured from a blank quartz plate. Decays were recorded to 5000 counts in the peak channel with a record length of 1024 channels with a signal count rate of 10 MHz. Iterative reconvolution of the IRF with one decay function and non-linear least-squares analysis were used to analyze the data. In all cases, the residuals are randomly distributed around zero and the χ^2 values are close to unity, indicating the satisfactory fitting quality for all decays.

Two-photon Absorption Measurements. TPA cross sections were determined via two-photon-excited fluorescence (TPEF) method by using coumarin 485 in methanol

as standard.[3] TPA cross section were δ_{TPA} measured on the basis of Equation (3).[4]

$$\delta_s = \delta_r \times \frac{\Phi_r}{\Phi_s} \times \frac{c_r}{c_s} \times \frac{n_r}{n_s} \times \frac{F_s}{F_r} \quad (3)$$

where c and n are the concentration and refractive index of the sample solution, respectively, F is the TPEF integral intensity and Φ is the quantum yield, the subscript r and s mean the reference and experimental sample, respectively.

The TPEF emission spectra were measured on a Princeton Instrument SpectroPro HRS-300S in conjunction with a CCD detector (Princeton Instrument PRO16×2B×3) as the recorder, and the pump laser beam came from a mode-locked Ti:sapphire laser system (Coherent Chameleon Ultra II, 680-1080 nm) with a pulse duration of 130 fs and a repetition rate of 80 MHz, respectively. The laser beam was focused into the sample (C = 2.0 × 10^{-5} M) by a lens. The power of laser was tuned by a filter and checked by a power meter after change wavelength of laser to make sure every spectrum was excited at the same laser power. The frequency up-converted fluorescence was collected at a direction perpendicular to the pump beam. To minimize there-absorption, the excitation beam was focused as closely as possible to the quartz cell wall, which faced the slit of spectrometer.

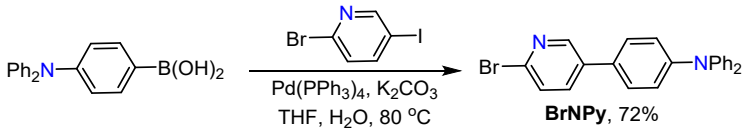
Synthesis

5-(2-Pyridyl)[6]helicene (Py-HC): To a mixture of **Bpin-HC** (160 mg, 0.35 mmol), K_2CO_3 (242 mg, 1.75 mmol) and $PdCl_2$(dppf) (26 mg, 0.035 mmol) were added degassed THF (12 mL) and H_2O (3 mL) under a steam of nitrogen. Subsequently, 2-bromopyridine (40 μL, 0.42 mmol) was added and the reaction mixture was heated at 80 °C in an oil bath overnight. The mixture was cooled to room temperature and then extracted with CH_2Cl_2. The combined organic layer was dried over anhydrous Na_2SO_4, filtered, and concentrated under reduced pressure. The resulted residue was purified by a silica gel column chromatography (5/1 petroleum ether/ethyl acetate, R_f = 0.50) to afford **Py-HC** (58 mg, 0.14 mmol) in 41% yield as yellow solids. mp 179.9–180.4 °C; ^{1}H NMR (400 MHz, $CDCl_3$) δ 8.92 (d, J = 4.0 Hz, 1H), 8.13 (s, 1H), 8.05–8.00 (m, 5H), 7.94 (s, 2H), 7.90 (td, J = 7.6, 2.0 Hz, 1H), 7.84 (d, J = 7.6 Hz, 1H), 7.79 (d, J = 7.6 Hz, 1H), 7.75 (d, J = 8.4 Hz, 1H), 7.73 (d, J = 8.0 Hz, 1H), 7.41 (ddd, J = 7.4, 4.8, 0.9 Hz, 1H), 7.25 (td, J = 7.2, 0.8 Hz, 1H), 7.20 (td, J = 7.2, 1.2 Hz, 1H), 6.79 (td, J = 7.2, 1.2 Hz, 1H), 6.70 (td, J = 7.2, 1.2 Hz, 1H); ^{13}C{^{1}H} NMR (100 MHz, $CDCl_3$) δ 159.1, 149.9, 138.0, 136.6, 133.6, 131.9, 131.5, 130.7, 130.6, 130.0, 129.9, 128.4,

128.22, 128.15, 128.1, 127.9, 127.8, 127.63, 127.58, 127.57, 127.4, 127.1, 126.3, 125.9, 125.7, 125.5, 125.4, 125.0, 124.8, 124.0, 122.3; HRMS (ESI) m/z: $[M+H]^+$ Calcd for $C_{31}H_{20}N$: 406.1590; Found 406.1588.

PhBPy-HC: Py-HC (58 mg, 0.14 mmol) was dissolved in dry CH_2Cl_2 (5 mL) in a 25 mL Schlenk tube and *i*-Pr_2NEt (20 μL, 0.14 mmol) was added under a nitrogen atmosphere. The mixture was cooled to 0 °C and BBr_3 (1.0 M in Hexane, 0.42 mL, 0.42 mmol) was added dropwise. The reaction mixture was brought to room temperature and it was stirred for 24 h at this temperature. After evaporation of the solvent under high vacuum, the residue was redissolved in toluene (6 mL). PhMgBr (1.0 M in THF, 1.7 mL, 1.7 mmol) was added dropwise under a steam of nitrogen. After the mixture was stirred at room temperature for 12 h, H_2O and CH_2Cl_2 were added successively. The resulting mixture was separated and the aqueous phase was extracted with CH_2Cl_2. The combined organic layer was dried over anhydrous Na_2SO_4, filtered, and concentrated under reduced pressure. The residue was purified by a silica gel column chromatography (2/1 petroleum ether/CH_2Cl_2, R_f = 0.30) to afford **PhBPy-HC** (41 mg, 0.072 mmol) in 51% yield as green solids. mp 319.3–320.1 °C; ^1H NMR (400 MHz, CD_2Cl_2) δ 8.68 (s, 1H), 8.63 (d, *J* = 8.0 Hz, 1H), 8.59 (d, *J* = 6.0 Hz, 1H), 8.16 (t, *J* = 7.8 Hz, 1H), 8.07–8.02 (m, 4H), 7.96 (s, 2H), 7.86 (d, *J* = 8.0 Hz, 1H), 7.67 (d, *J* = 8.4 Hz, 1H), 7.45 (t, *J* = 6.6 Hz, 1H), 7.40 (d, *J* = 8.4 Hz, 1H), 7.34–7.27 (m, 5H), 7.22 (d, *J* = 6.4 Hz, 1H), 7.05 (d, *J* = 6.8 Hz, 1H), 7.03–6.95 (m, 3H), 6.86 (d, *J* = 7.8 Hz, 2H), 6.71 (t, *J* = 7.8 Hz, 1H), 6.65 (t, *J* = 7.2 Hz, 1H); $^{13}C\{^1H\}$ NMR (100 MHz, CD_2Cl_2) δ 153.9, 147.9, 140.6, 135.4, 134.6, 133.2, 132.4, 132.3, 131.82, 131.77, 130.6, 130.2, 129.0, 128.8, 128.7, 128.6, 128.5, 128.2, 127.99, 127.96, 127.7, 127.5, 127.4, 127.3, 127.2, 126.5, 126.2, 126.1, 125.92, 125.85, 125.3, 125.2, 124.8, 124.29, 124.25, 123.1; ^{11}B NMR (128 MHz, CD_2Cl_2) δ 0.6; HRMS (ESI) m/z: $[M+K]^+$ Calcd for $C_{43}H_{28}BKN$: 608.1946; Found 608.1946.

Scheme S1



2-Bromo-5-[4-(N,N-diphenylamino)phenyl]pyridine (BrNPy): This compound was prepared essentially in the same manner as described for **Py-HC** using 4-(*N*,*N*-diphenylamino)phenylboronic acid (1.73 g, 6.00 mmol), 2-bromo-5-iodopyridine (2.20 g, 7.80 mmol), K_2CO_3 (2.50 g, 18.0 mmol), $Pd(PPh_3)_4$ (0.69 g, 0.60 mmol), degassed

THF (60 mL) and H_2O (15 mL). The purification by a silica gel column chromatography (10/1 petroleum ether/ethyl acetate, R_f = 0.50) afforded **BrNPy** (1.80 g, 4.32 mmol) in 72% yield as white solids. mp 146.6–147.0 °C; ^{1}H NMR (400 MHz, $CDCl_3$) δ 8.56 (d, *J* = 2.4 Hz, 1H), 7.70 (dd, *J* = 8.4, 2.4 Hz, 1H), 7.51 (d, *J* = 8.4 Hz, 1H), 7.40 (d, *J* = 8.8 Hz, 2H), 7.29 (t, *J* = 7.2 Hz, 4H), 7.17–7.11 (m, 6H), 7.07 (t, *J* = 7.2 Hz, 2H); ^{13}C{^{1}H} NMR (100 MHz, $CDCl_3$) δ 148.5, 148.1, 147.4, 140.2, 136.4, 135.6, 129.7, 129.5, 128.0, 127.8, 125.0, 123.6, 123.4; HRMS (ESI) m/z: $[M+H]^+$ Calcd for $C_{23}H_{18}BrN_2$: 401.0648; Found 401.0642.

Mixture of BPin-HC and BiBPin-HC: To a mixture of **DiBr-HC** (340 mg, 0.70 mmol), B_2Pin_2 (710 mg, 2.80 mmol), KOAc (412 mg, 4.20 mmol) and $PdCl_2$dppf (102 mg, 0.14 mmol) was added degassed 1,4-dioxane (25 mL) under a steam of nitrogen. The reaction mixture was heated at 100 °C in an oil bath overnight. The mixture was cooled to room temperature and then extracted with EtOAc. The combined organic layer was dried over anhydrous Na_2SO_4, filtered, and concentrated under reduced pressure. The residue was purified by a silica gel column chromatography (3/1 petroleum ether/CH_2Cl_2, R_f = 0.30 and 0.20) to afford the mixture of **BPin-HC** and **BiBPin-HC** (230 mg) as yellow solids. This mixture was used directly in the next step reaction without further separation. Based on comparison of ^{1}H NMR spectra between the mixture and the pure **BPin-HC** (Fig. S1), the molar ratio of **BPin-HC** to **BiBPin-HC** was determined to be about 1:1.4.

5-{5-[4-(N,N-diphenylamino)phenyl]-2-pyridyl}[6]helicene (NPy-HC) and 5,12-bis{5-[4-(N,N-diphenylamino)phenyl]-2-pyridyl}[6]helicene (BiNPy-HC): To a mixture of **Bpin-HC** and **BiBpin-HC** (230 mg), **BrNPy** (515 mg, 1.28 mmol), K_3PO_4 (657 mg, 3.10 mmol), Pd_2dba_3 (47 mg, 0.050 mmol) and Sphos (42 mg, 0.10 mmol) were added degassed DMF (10 mL) and H_2O (2.5 mL) under a steam of nitrogen. The reaction mixture was heated at 90 °C in an oil bath overnight. The mixture was cooled to room temperature and then extracted with EtOAc. The combined organic layer was dried over anhydrous Na_2SO_4, filtered, and concentrated under reduced pressure. The resulted residue was purified by a silica gel column chromatography to afford **NPy-HC** (5/1 petroleum ether/ethyl acetate, R_f = 0.50, 95 mg, 0.15 mmol) and **BiNPy-HC** (3/1 petroleum ether/ethyl acetate, R_f = 0.30, 81 mg, 0.084mmol) in 21% and 12% overall yields of two steps, respectively. They both were obtained as yellow-green solids. **NPy-HC**: mp 236.1–237.0 °C. ^{1}H NMR (400 MHz, $CDCl_3$) δ 9.12 (d, *J* = 1.6 Hz, 1H), 8.19 (s, 1H), 8.12 (d, *J* = 7.6 Hz, 1H), 8.07 (dd, *J* = 8.0, 2.4 Hz, 1H), 8.04 (s, 2H), 8.02–7.99 (m, 2H), 7.96 (d, *J* = 8.8 Hz, 1H), 7.94 (d, *J* = 8.8 Hz, 1H), 7.85 (d, *J* = 8.0 Hz, 1H),

7.84 (d, *J* = 7.2 Hz, 1H), 7.73 (t, *J* = 9.0 Hz, 2H), 7.63–7.60 (m, 2H), 7.32 (t, *J* = 7.8 Hz, 4H), 7.25–7.19 (m, 8H), 7.09 (t, *J* = 7.4 Hz, 2H), 6.79 (ddd, *J* = 8.4, 7.0, 1.6 Hz, 1H), 6.70 (ddd, *J* = 8.4, 7.2, 1.2 Hz, 1H); ^{13}C NMR (101 MHz, $CDCl_3$) δ 157.1, 148.2, 147.8, 147.5, 137.6, 134.6, 134.2, 133.6, 131.9, 131.4, 131.0, 130.7, 130.6, 129.94, 129.86, 129.5, 128.4, 128.19, 128.15, 128.1, 127.94, 127.87, 127.7, 127.62, 127.56, 127.4, 127.1, 126.3, 125.9, 125.7, 125.5, 125.3, 125.0, 124.9, 124.8, 124.0, 123.7, 123.5; HRMS (ESI) m/z: $[M+H]^+$ Calcd for $C_{49}H_{33}N_2$: 649.2638; Found 649.2635. **BiNPy-HC:** mp 301.8–302.6 °C; ^{1}H NMR (400 MHz, $CDCl_3$) δ 9.12 (s, 2H), 8.20 (s, 2H), 8.14–8.07 (m, 8H), 7.87 (d, *J* = 7.2 Hz, 4H), 7.62 (d, *J* = 8.0 Hz, 4H), 7.32 (t, *J* = 7.4 Hz, 8H), 7.23–7.18 (m, 14H), 7.09 (t, *J* = 7.2 Hz, 4H), 6.81 (t, *J* = 7.4 Hz, 2H); ^{13}C{^{1}H} NMR (100 MHz, $CDCl_3$) δ 157.1, 148.2, 147.8, 147.6, 137.8, 134.7, 134.3, 131.1, 130.8, 130.7, 129.9, 129.6, 128.5, 128.4, 127.9, 127.83, 127.75, 127.5, 126.0, 125.5, 125.4, 125.1, 124.9, 123.7, 123.5; HRMS (ESI) m/z: $[M+H]^+$ Calcd for $C_{72}H_{49}N_4$: 969.3952; Found 969.3948.

NPhBPy-HC: This compound was prepared essentially in the same manner as described for **PhBPy-HC** using **NPy-HC** (60 mg, 0.092 mmol), CH_2Cl_2 (5 mL), *i*-Pr_2NEt (13 μL, 0.092 mmol), BBr_3 (1.0 M in Hexane, 0.28 mL, 0.28 mmol), toluene (6 mL), and PhMgBr (1.0 M in THF, 1.1 mL, 1.1 mmol). The borylative cyclization with BBr_3 and subsequent quenching of the dibromoborane intermediates with PhMgBr were carried out at 60 °C and room temperature, respectively. The purification by a silica gel column chromatography (5/1 petroleum ether/ethyl acetate, R_f = 0.20) to afforded **NPhBPy-HC** (27 mg, 0.033 mmol) in 36% yield as yellow solids. mp 326.9–328.0 °C; ^{1}H NMR (400 MHz, $CDCl_3$) δ 8.85 (s, 1H), 8.65 (d, *J* = 8.8 Hz, 1H), 8.63 (s, 1H), 8.26 (d, *J* = 8.4 Hz, 1H), 8.02–7.92 (m, 6H), 7.81 (d, *J* = 7.6 Hz, 1H), 7.66 (d, *J* = 8.4 Hz, 1H), 7.40 (d, *J* = 8.4 Hz, 1H), 7.35–7.28 (m, 10H), 7.24–7.18 (m, 2H), 7.15–7.00 (m, 14H), 6.67 (t, *J* = 7.6 Hz, 2H); ^{13}C{^{1}H} NMR (100 MHz, $CDCl_3$) δ 151.3, 149.3, 147.2, 145.3, 137.0, 135.1, 134.8, 134.2, 133.6, 132.06, 132.04, 131.9, 131.5, 130.3, 129.9, 129.7, 128.9, 128.7, 128.6, 128.30, 128.25, 128.0, 127.8, 127.60, 127.58, 127.55, 127.3, 127.20, 127.16, 127.1, 126.9, 126.2, 125.93, 125.88, 125.5, 125.34, 125.29, 125.2, 125.1, 124.7, 124.0, 123.6, 123.0; ^{11}B NMR (128 MHz, $CDCl_3$) δ 2.9; HRMS (ESI) m/z: $[M+K]^+$ Calcd for $C_{61}H_{41}BKN_2$: 851.2994; Found 851.2990.

NFBPy-HC: This compound was prepared essentially in the same manner as described for **PhBPy-HC** using **NPy-HC** (68 mg, 0.10 mmol), CH_2Cl_2 (5 mL), *i*-Pr_2NEt (14 μL, 0.10 mmol), BBr_3 (1.0 M in Hexane, 0.30 mL, 0.30 mmol), toluene (6 mL) and C_6F_5MgBr (0.8 M in Et_2O, 1.5 mL, 1.2 mmol). The borylative cyclization with BBr_3

and subsequent quenching of the dibromoborane intermediates with C_6F_5MgBr were carried out at 60 °C and room temperature, respectively. The purification by a silica gel column chromatography (3/1 petroleum ether/ethyl acetate, R_f = 0.40) afforded **NFBPy-HC** (28 mg, 0.028 mmol) in 28% yield as orange solids. mp 204.2–205.0 °C; (*M*)-**NFBPy-HC**: $[\alpha]^{25}$ = +485.9; (*P*)-**NFBPy-HC**: $[\alpha]^{25}$ = –501.6; ^{1}H NMR (400 MHz, CD_2Cl_2) δ 8.91 (d, *J* = 2.0 Hz, 1H), 8.78 (s, 1H), 8.70 (d, *J* = 8.8 Hz, 1H), 8.36 (dd, *J* = 8.8, 2.4 Hz, 1H), 8.11 (d, *J* = 8.0 Hz, 1H), 8.08 (d, *J* = 8.0 Hz, 1H), 8.07 (d, *J* = 8.4 Hz, 1H), 8.04 (d, *J* = 8.4 Hz, 1H), 7.97 (d, *J* = 8.8 Hz, 1H), 7.95 (d, *J* = 9.2 Hz, 1H), 7.84 (d, *J* = 7.6 Hz, 1H), 7.63 (d, *J* = 8.4 Hz, 1H), 7.46 (dd, *J* = 8.2, 0.8 Hz, 1H), 7.40 (d, *J* = 8.7 Hz, 2H), 7.34 (t, *J* = 7.9 Hz, 4H), 7.26 (d, *J* = 7.2 Hz, 1H), 7.32 (t, *J* = 8.0 Hz, 1H), 7.17–7.11 (m, 8H), 6.64 (t, *J* = 7.8 Hz, 2H); $^{13}C\{^1H\}$ NMR (100 MHz, CD_2Cl_2) δ 151.0, 149.9, 147.3, 143.6, 139.0, 136.9, 134.8, 132.4, 132.2, 131.9, 130.6, 129.94, 129.92, 129.88, 129.4, 128.9, 128.7, 128.6, 128.2, 128.0, 127.9, 127.7, 127.6, 127.2, 126.93, 126.90, 126.5, 126.19, 126.16, 126.1, 126.0, 125.8, 125.2, 124.6, 124.5, 124.3, 122.8; ^{11}B NMR (128 MHz, $CDCl_3$) δ –3.9; ^{19}F NMR (377 MHz, CD_2Cl_2) δ –130.63 (dd, *J* = 23.7, 7.1 Hz, 2F), –132.59 (dd, *J* = 23.9, 6.8 Hz, 2F), –158.38 (t, *J* = 20.3 Hz, 1F), –159.20 (t, *J* = 20.5 Hz, 1F), –164.18 (td, *J* = 22.2, 8.3 Hz, 2F), –164.37 (td, *J* = 22.2, 8.3 Hz, 2F); HRMS (ESI) m/z: $[M+H]^+$ Calcd for $C_{61}H_{32}BF_{10}N_2$: 993.2493; Found 993.2471.

BiNFBPy-HC: This compound was prepared essentially in the same manner as described for **PhBPy-HC** using **BiNPy-HC** (60 mg, 0.060 mmol), CH_2Cl_2 (6 mL), *i*-Pr_2NEt (17 μL, 0.12 mmol), BBr_3 (1.0 M in Hexane, 0.36 mL, 0.36 mmol), toluene (8 and C_6F_5MgBr (0.8 M in Et_2O, 1.5 mL, 1.2 mmol). The borylative cyclization with BBr_3 and subsequent quenching of the dibromoborane intermediates with C_6F_5MgBr were carried out at 60 °C and 90 °C, respectively. The purification by a silica gel column chromatography (2/1 petroleum ether/ethyl acetate, R_f = 0.30) afforded **BiNFBPy-HC** (31 mg, 0.019 mmol) of in 31% yield as orange solids. mp 270.8–271.3 °C; (*M*)-**BiNFBPy-HC**: $[\alpha]^{25}$ = +420.1; (*P*)-**BiNFBPy-HC**: $[\alpha]^{25}$ = –408.0; ^{1}H NMR (400 MHz, CD_2Cl_2) δ 8.92 (d, *J* = 2.0 Hz, 2H), 8.79 (s, 2H), 8.72 (d, *J* = 8.8 Hz, 2H), 8.41 (dd, *J* = 8.6, 1.6 Hz, 2H), 8.18 (d, *J* = 8.0 Hz, 2H), 8.11 (d, *J* = 8.4 Hz, 2H), 7.57 (d, *J* = 8.4 Hz, 2H), 7.41 (d, *J* = 8.4 Hz, 4H), 7.33 (t, *J* = 7.8 Hz, 8H), 7.24 (d, *J* = 6.8 Hz, 2H), 7.16–7.11 (m, 16H), 6.65 (t, *J* = 7.8 Hz, 2H); $^{13}C\{^1H\}$ NMR (100 MHz, CD_2Cl_2) δ 150.9, 150.0, 147.3, 143.6, 139.0, 137.1, 136.1, 132.5, 131.0, 130.4, 130.0, 129.1, 128.0, 127.8, 126.92, 126.86, 126.60, 126.55, 126.4, 125.8, 124.8, 124.6, 124.2, 122.8; ^{11}B NMR (128 MHz, $CDCl_3$) δ –4.7; ^{19}F NMR (377 MHz, CD_2Cl_2) δ –130.65 (dd, *J* = 23.8,

6.4 Hz, 4F), –132.65 (dd, J = 24.0, 6.8 Hz, 4F), –158.09 (t, J = 20.4 Hz, 2F), –159.27 (t, J = 20.4 Hz, 2F), –163.87 (td, J = 22.1, 8.3 Hz, 4F), –164.45 (td, J = 22.2, 8.3 Hz, 4F); MALDI-TOF (MS) m/z: $[M]^{\bullet+}$ Calcd for $C_{96}H_{46}B_2F_{20}N_4$: 1656.3589; Found 1656.3691.

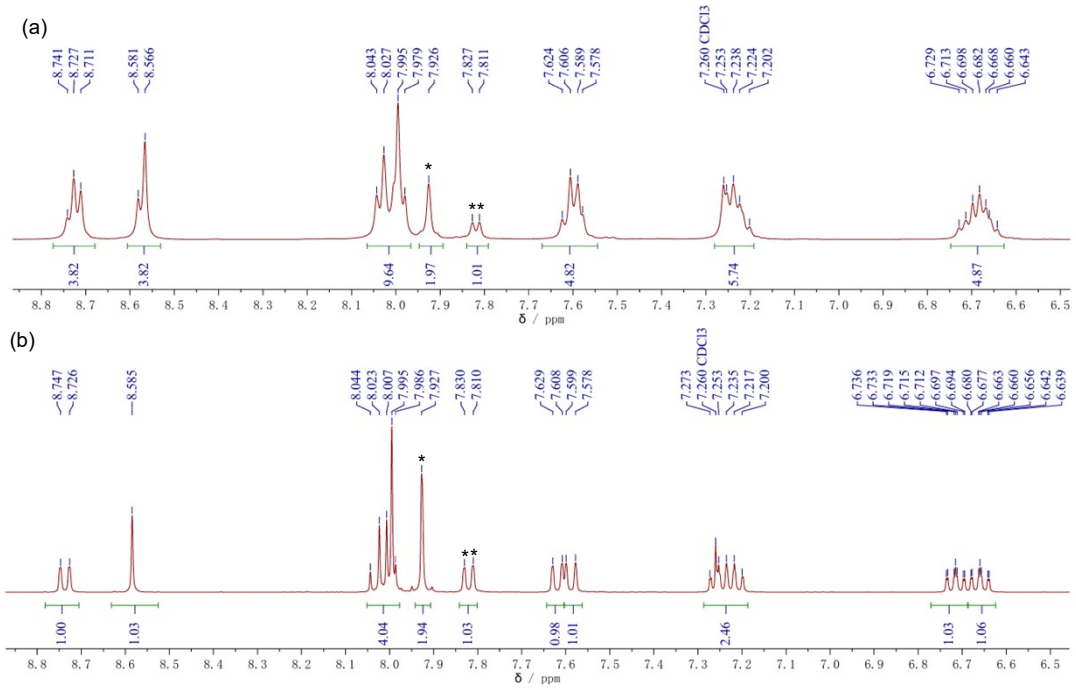


Fig. S1 ^{1}H NMR spectra for the aromatic region of (a) the mixture of **BPin-HC** and **BiBPin-HC** (500M, $CDCl_3$), and **BPin-HC** (400M, $CDCl_3$)[1].

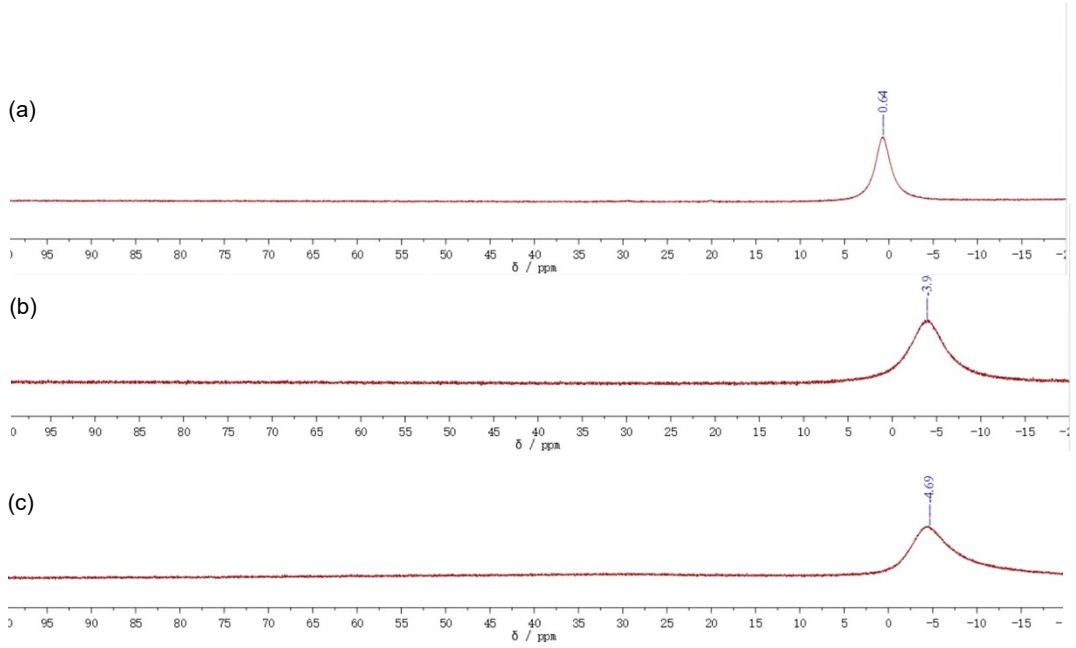


Fig. S2 ^{11}B NMR spectra (128 M Hz) of (a) **PhBPy-HC** (CD_2Cl_2), (b) **NFBPy-HC** ($CDCl_3$), and (c) **BiNFBPy-HC** ($CDCl_3$).

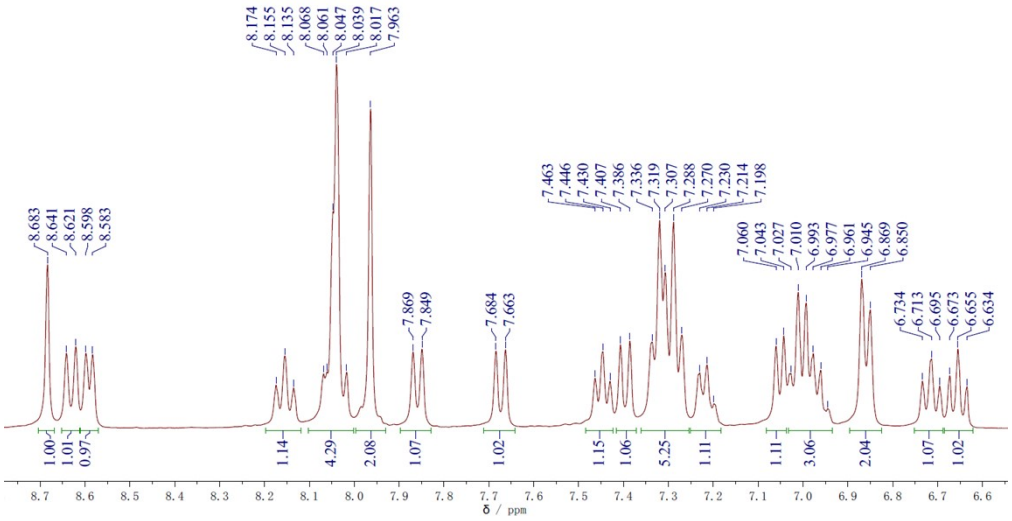


Fig. S3 ^{1}H NMR spectra (400 MHz) for the aromatic region of **PhBPy-HC** (CD_2Cl_2).

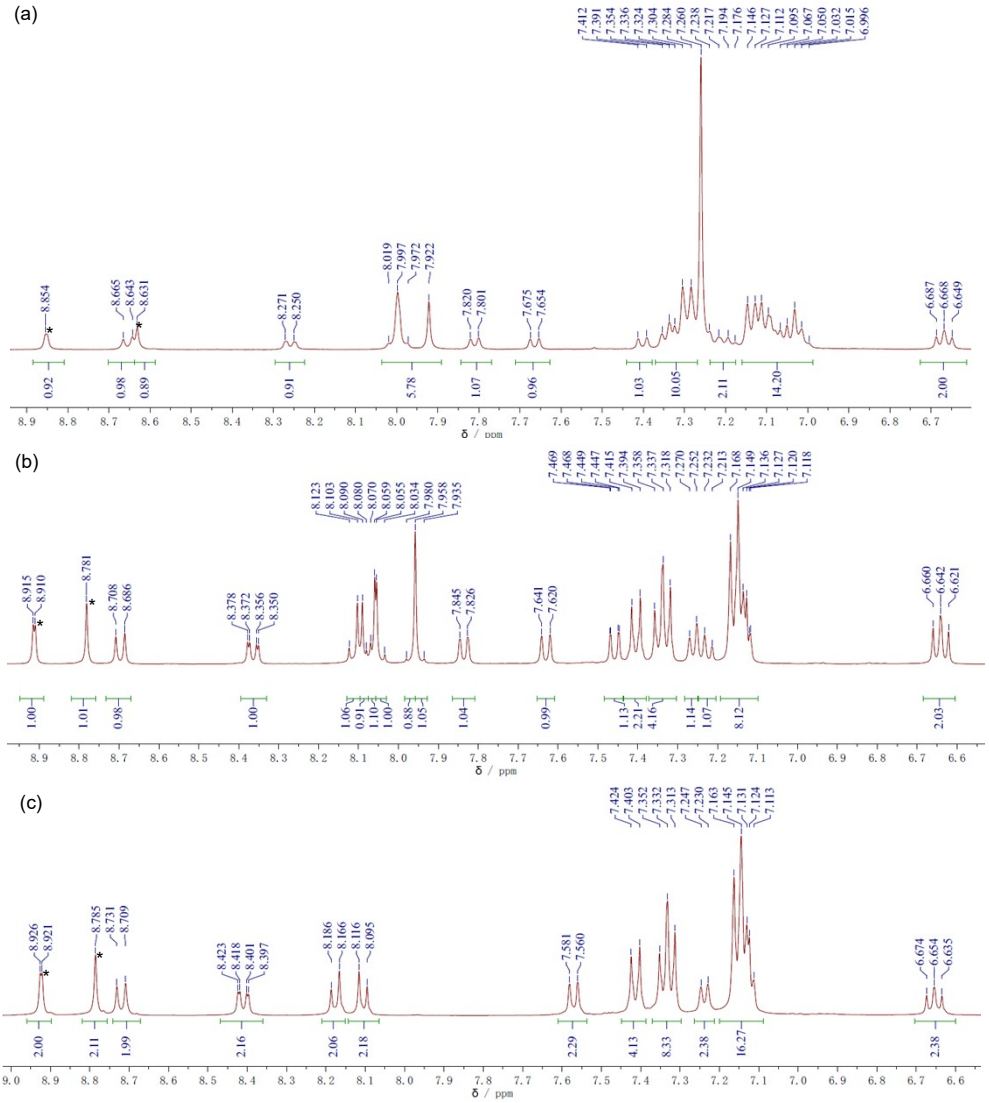


Fig. S4 ^{1}H NMR spectra (400 MHz) for the aromatic region of (a) **NPhBPy-HC** ($CDCl_3$), (b) **NFBPy-HC** (CD_2Cl_2), and (c) **BiNFBPy-HC** (CD_2Cl_2).

X-ray Crystal Structure Analysis[5]

Table S1 Crystal data of **PhBPy-HC** (CCDC: 2488475) and **NFBPy-HC** (CCDC: 2488477).

	PhBPy-HC	**NFBPy-HC**
Empirical formula	$C_{43}H_{28}BN$	$C_{62}H_{32}BCl_3F_{10}N_2$
Formula weight	569.47	1112.05
Temperature/K	173.00	173.00
Crystal system	triclinic	monoclinic
Space group	*P*1	$P2_1/c$
a/Å	14.347(3)	27.5353(16)
b/Å	14.439(3)	13.9114(7)
c/Å	15.615(3)	12.6024(7)
α/°	105.046(12)	90
β/°	92.561(12)	94.797(3)
γ/°	108.743(11)	90
Volume/Å^3	2929.1(10)	4810.5(5)
Z	4	4
ρ_{calc}g/cm^3	1.291	1.535
μ/mm^{-1}	0.560	2.468
F(000)	1192	2256
Crystal size/mm^3	0.08 × 0.06 × 0.05	0.12 × 0.06 × 0.05
Radiation	CuKα (λ = 1.54178)	CuKα (λ = 1.54178)
2θ range for data collection/°	2.959 to 66.593	1.610 to 66.595
Reflections collected	22605	33302
Independent reflections	10122 [R_{int} = 0.1028, R_{sigma} = 0.1795]	8425 [R_{int} = 0.1078, R_{sigma} = 0.1045]
Data/restraints/parameters	10122/0/812	8425/153/703
Goodness-of-fit on F^2	0.939	0.983
Final R indexes [I>=2σ(I)]	R_1 = 0.0920, wR_2 = 0.2226	R_1 = 0.1067, wR_2 = 0.2976
Final R indexes [all data]	R_1 = 0.1842, wR_2 = 0.3138	R_1 = 0.1297, wR_2 = 0.3242
Largest diff. peak/hole/e Å^{-3}	0.389/–0.335	1.007/–1.224

PhBPy-HC: The single crystal was obtained by diffusion of hexane into $CHCl_3$ solutions. Intensity data were collected at 173 K on a Bruker SMART CCD X-ray Diffractometer (APEX II) with Cu Kα radiation (λ = 1.54178 Å) and graphite monochrometer.

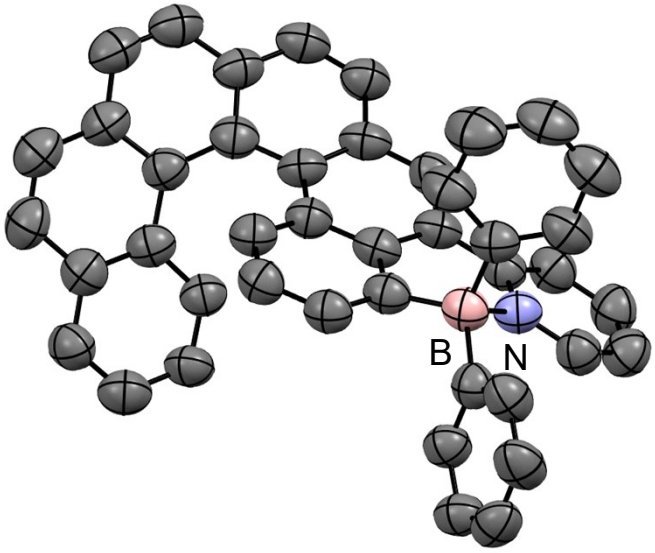


Fig. S5 Thermal ellipsoidal plot of **PhBPy-HC**. All ellipsoids are drawn at the 50% probability level, and H atoms are omitted for clarity.

NFBPy-HC: The single crystal was obtained by diffusion of methanol into $CHCl_3$ solutions. Intensity data were collected at 173 K on a Bruker SMART CCD X-ray Diffractometer (APEX II) with Cu Kα radiation (λ = 1.54178 Å) and graphite monochrometer.

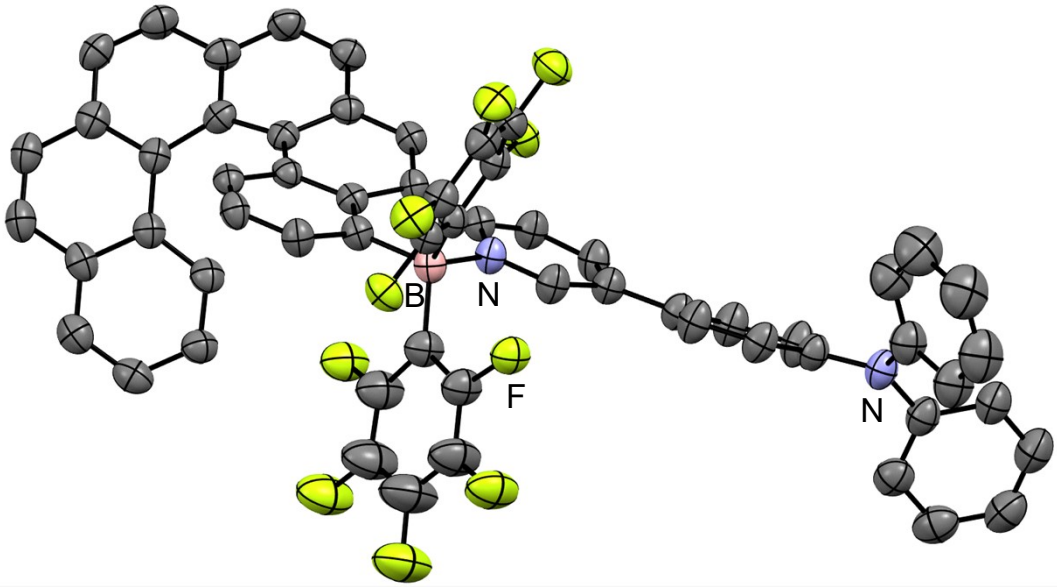


Fig. S6 Thermal ellipsoidal plot of **NFBPy-HC**. All ellipsoids are drawn at the 50% probability level, and H atoms are omitted for clarity.

Optical Resolution of NFBPy-HC and BiNFBPy-HC

Preparative Separation Method of NFBPy-HC

The enantiomer was separated by chiral HPLC [ChiralPak IA, DCM/MeOH = 50:50, flow rate = 50 mL/min, λ = 220 nm, 25 °C].

Analytical Separation Method of NFBPy-HC

Enantiomeric purity was determined by chiral HPLC analysis [ChiralPak IA, DCM/MeOH = 30:70, flow rate = 1.0 mL/min, λ = 220 nm, 35 °C], t_{R1} = 5.933 min, t_{R2} = 6.897 min.

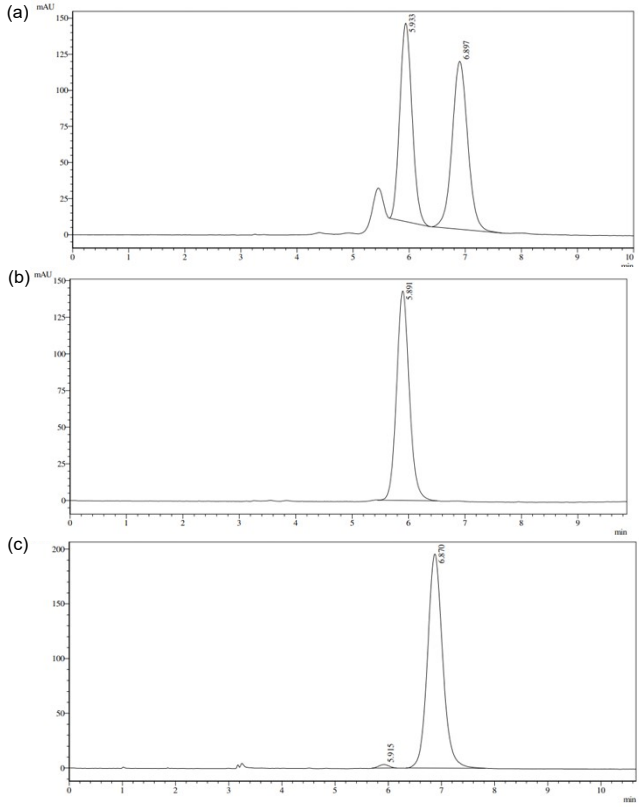


Fig. S7 Chiral HPLC profiles of (a) *rac*-**NFBPy-HC**, (b) (*P*)-(–)-**NFBPy-HC**, and (c) (*M*)-(+)-**NFBPy-HC**.

Table S2 The HPLC profiles of **NFBPy-HC**.

	Fraction	Retention Time/min	Area	Area%	ee
rac-form	(*P*)-isomer	5.933	2098523	48.22	-
	(*M*)-isomer	6.897	2253319	51.78	-
(*P*)-isomer	(*P*)-isomer	5.891	2246098	100	>99%
	(*M*)-isomer	-	-	-	
(*M*)-isomer	(*P*)-isomer	5.915	42266	1.08	
	(*M*)-isomer	6.870	3868792	98.92	>97%

Preparative Separation Method of BiNFBPy-HC

The enantiomer was separated by chiral HPLC [ChiralPak IA, DCM/MeOH = 50:50, flow rate = 50 mL/min, λ = 254 nm, 25 °C].

Analytical Separation Method of BiNFBPy-HC

Enantiomeric purity was determined by chiral HPLC analysis [ChiralPak IA, DCM/MeOH = 50:50, flow rate = 1.0 mL/min, λ = 254 nm, 35 °C], t_{R1} = 4.257 min, t_{R2} = 5.335 min.

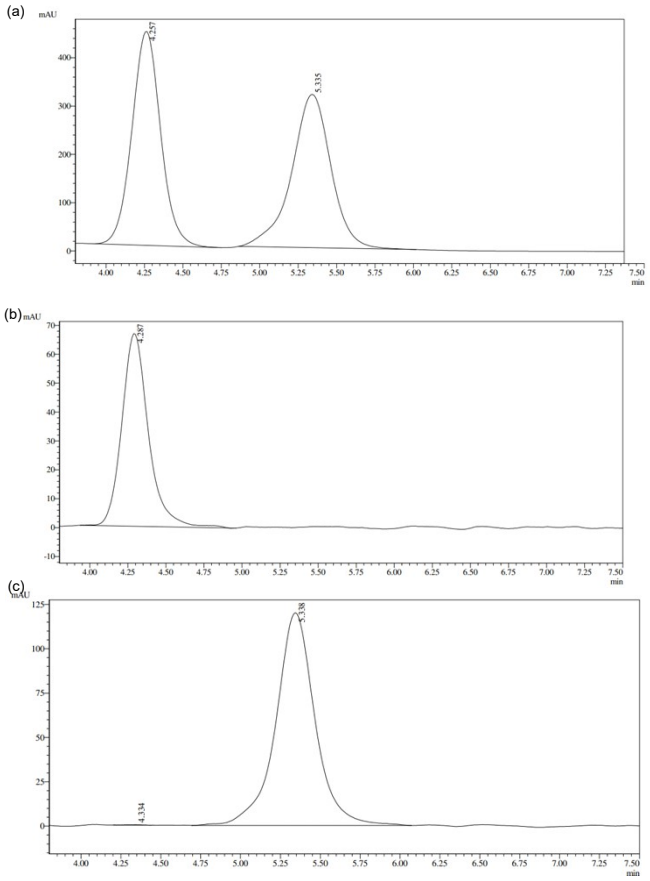


Fig. S8 Chiral HPLC profiles of (a) *rac*-**BiNFBPy-HC**, (b) (*P*)-(−)-**BiNFBPy-HC**, and (c) (*M*)-(+)-**BiNFBPy-HC**.

Table S3 The HPLC profiles of **BiNFBPy-HC**

	Fraction	Retention Time/min	Area	Area%	ee
rac-form	(*P*)-isomer	4.257	5766884	50.51	-
	(*M*)-isomer	5.335	5649793	49.487	-
(*P*)-isomer	(*P*)-isomer	4.287	811780	100	>99%
	(*M*)-isomer	-	-	-	
(*M*)-isomer	(*P*)-isomer	4.334	878	0.043	
	(*M*)-isomer	5.338	2058629	99.957	>99%

Photophysical Properties

Table S4 Photophysical properties in various solvents.

		λ_{abs}/nm (ε/10^4 M^{-1} cm^{-1})[a]	λ_{em}/nm	FWHM/nm	Φ_F[b]
PhBPy-HC	cyclohexane	419 (1.72), 455 (0.68)	489	62	0.25
	toluene	416 (1.90), 454 (0.55)	491	66	0.32
	$CHCl_3$	416 (1.61), 453 (0.46)	492	66	0.21
	THF	410 (2.44), 453 (0.44)	491	67	0.23
NPhBPy-HC	cyclohexane	435 (3.77), 463 (2.67)	493, 515	54	0.45
	toluene	437 (3.62), 461 (2.81)	495, 517	56	0.33
	$CHCl_3$	436 (3.84), 461 (2.98)	500	63	0.34
	THF	434 (3.83), 456 (3.04)	526	83	0.28
NFBPy-HC	cyclohexane	444 (4.19), 470 (3.70)	493, 522	48	0.49
	toluene	445 (3.85), 468 (3.47)	508	58	0.48
	$CHCl_3$	444 (3.74), 466 (3.36)	533	68	0.35
	THF	442 (3.71), 461 (3.29)	553	87	0.12
BiNFBPy-HC	cyclohexane	451 (8.09), 468 (8.84)	496, 525	28	0.41
	toluene	448 (5.55), 465 (6.10)	511	59	0.39
	$CHCl_3$	447 (5.70), 465 (6.37)	533	70	0.26
	THF	442 (6.68), 461 (7.45)	555	88	0.10

[a]Only the longest maxima are shown. [b]Calculated using coumarin 307 as a standard.

Table S5 Fluorescence lifetime in cyclohexane and powder.

		τ_1/ns (Rel %)	τ_2/ns (Rel %)	τ_3/ns (Rel %)	τ_{av}/ns[a]	χ^2
PhBPy-HC	cyclohexane	6.27 (100)	-	-	6.27	0.980
	powder	0.42 (10)	2.35 (36)	4.58 (54)	3.36	1.139
NPhBPy-HC	cyclohexane	3.57 (100)	-	-	3.57	1.158
	powder	0.45 (34)	1.37 (58)	4.11 (8)	1.28	1.198
NFBPy-HC	cyclohexane	2.48 (100)	-	-	2.48	1.093
	powder	0.51 (17)	2.22 (60)	5.92 (23)	2.78	1.007
BiNFBPy-HC	cyclohexane	2.31 (100)	-	-	2.31	1.131
	powder	0.27 (21)	1.33 (53)	4.54 (26)	1.94	1.072
BiNPy-HC	cyclohexane	9.82 (100)	-	-	9.82	1.182

[a]Average lifetime (τ_{av}) is calculated by the equation $\tau_{av} = \Sigma A_i\tau_i^2/\Sigma A_i\tau_i$, where A_i is the preexponential for lifetime τ_i.[6]

Chiroptical Properties

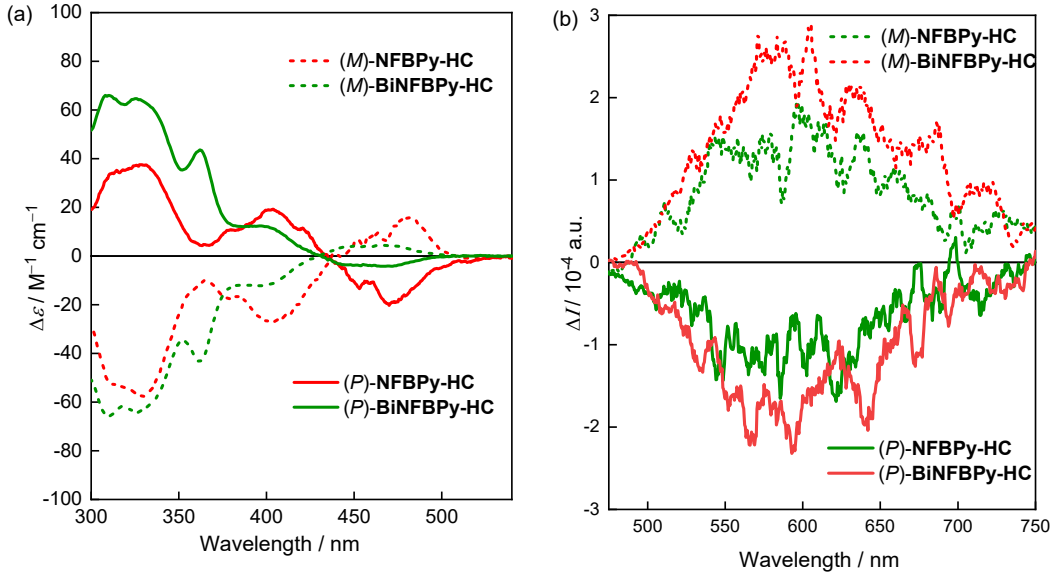


Fig. S9 (a) CD (c = 2.0 × 10^{-5} M) and (b) CPL (c = 2.0 × 10^{-5} M, λ_{ex} = 370 nm) spectra of **NFBPy-HC** and **BiNFBPy-HC** in THF.

Table S6 Chiroptical properties of **NFBPy-HC** and **BiNFBPy-HC** in THF.

	$\lvert g_{abs}\rvert/10^{-4}$	$\lvert g_{lum}\rvert/10^{-4}$	B_{CPL}/M^{-1} cm^{-1}
NFBPy-HC	1.65 (468)	2.64 (615)	0.63
BiNFBPy-HC	4.73 (479)	4.13 (605)	2.74

Theoretical Calculations

The ground-state geometries were optimized using Gaussian 16 with the density functional theory (DFT) method at PBE0-D3(BJ)/6-31G(d) level.[7] Based on the optimized ground state structure, the geometrical optimizations of the first excited state (S_1) were calculated by TD-DFT method at PBE0-D3(BJ)/6-31G(d) level. To ensure that the optimized geometry was at a minimum, all geometry optimizations were followed by a frequency calculation and only positive frequencies were obtained. The one-photon absorption (OPA) vertical transitions were calculated at B3LYP-D3(BJ)/6-31G(d) level, keeping consistence with the two-photon absorption (TPA) calculations. The molecular orbitals were visualized using GaussView 6.0 software. The simulated UV-Vis spectra and ECD spectra were generated by SpecDis 1.71 with a sigma of 0.20 eV.[8] The TPA calculation based on the optimized geometries was obtained using response theory at B3LYP-D3(BJ)/6-31G(d) level in Dalton 2021.[9] The simulated TPA spectra were generated by using the calculated transition energies and TPA probability

provided by the quadratic RF with a Gaussian line shape function.

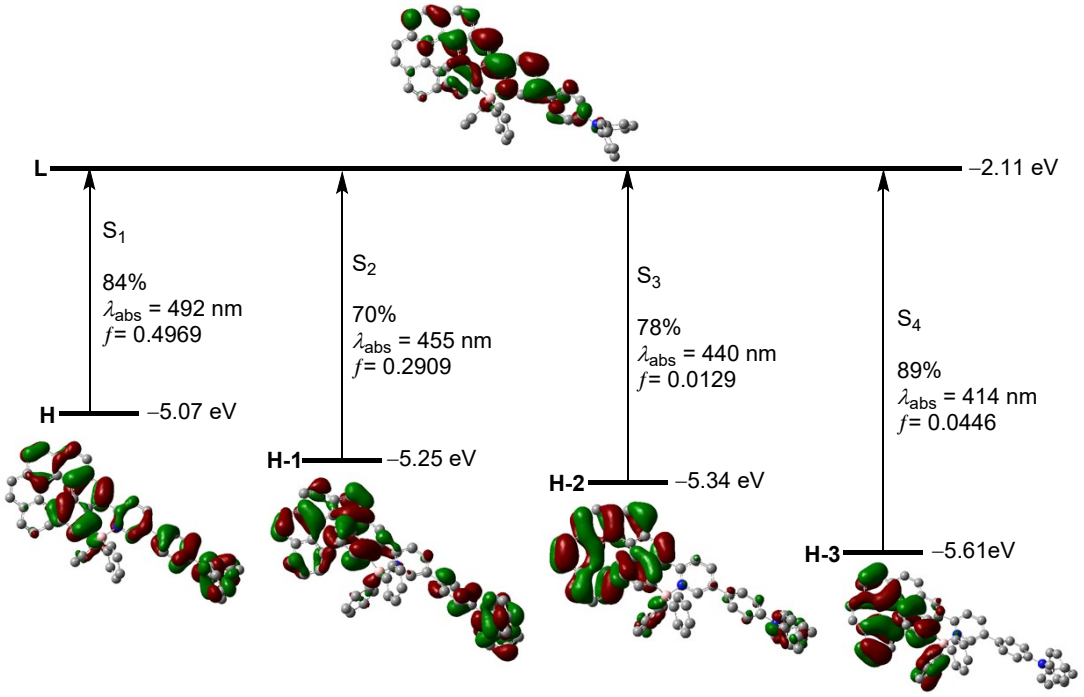


Fig. S10 Kohn–Sham energy levels, pictorial drawing of frontier orbitals, and transitions of **NPhBPy-HC** at the S_0 geometry, calculated at TD-B3LYP-D3(BJ)/6-31g(d) level.

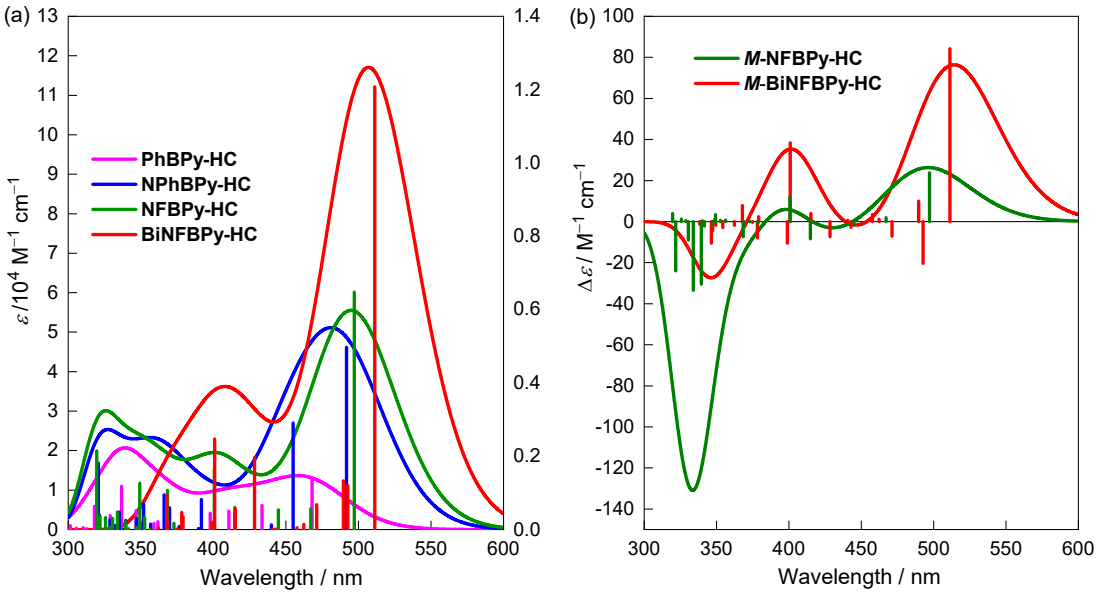


Fig. S11 (a) Calculated UV-vis spectrum of **PhBPy-HC**, **NPhBPy-HC**, **NFBPy-HC** and **BiNFBPy-HC**, and (b) calculated CD spectrum of (*M*)-**NFBPy-HC** and (*M*)-**BiNFBPy-HC**, calculated at TD-B3LYP-D3(BJ)/6-31G(d) level.

Table S7 Selected calculated wavelength, oscillator strength and compositions of major

transitions for all compounds calculated at TD-B3LYP-D3(BJ)/6-31G(d) level.

			OPA			TPA		
	transition	composition	*E*/ev	*λ*/nm	*f*	*λ*/nm	pro./10^4a.u.	*σ*/GM
PhBPy	$S_0 \rightarrow S_1$	H→L (94%)	2.65	468	0.1378	–	–	–
-HC	$S_0 \rightarrow S_2$	H-1→L (87%)	2.87	433	0.0660	–	–	–
	$S_0 \rightarrow S_3$	H-2→L (85%)	3.02	411	0.0500	–	–	–
	$S_0 \rightarrow S_4$	H-3→L (86%)	3.12	398	0.0447	–	–	–
NPhBPy	$S_0 \rightarrow S_1$	H→L (84%)	2.53	492	0.4969	984	0.231	10.7
-HC	$S_0 \rightarrow S_2$	H-1→L (70%)	2.73	455	0.2909	912	7.70	419
	$S_0 \rightarrow S_3$	H-2→L (78%)	2.82	440	0.0129	879	9.02	525
	$S_0 \rightarrow S_4$	H-3→L (89%)	2.99	414	0.0446	829	6.14	402
	$S_0 \rightarrow S_5$	H→L+1 (82%)	3.16	392	0.082	782	0.0157	1.15
NFBPy	$S_0 \rightarrow S_1$	H→L (88%)	2.50	497	0.6476	995	3.59	164
-HC	$S_0 \rightarrow S_2$	H-1→L (80%)	2.66	467	0.0565	935	8.53	440
	$S_0 \rightarrow S_3$	H-2→L (87%)	2.79	445	0.0537	888	9.04	514
	$S_0 \rightarrow S_4$	H-3→L (92%)	3.00	415	0.0603	829	3.68	241
	$S_0 \rightarrow S_5$	H→L+1 (93%)	3.09	400	0.1638	802	1.35	95
	$S_1 \rightarrow S_0$	H→L (85%)	2.18	570	0.5631	–	–	–
BiNFBPy	$S_0 \rightarrow S_1$	H-1→L (19%) H→L+1 (66%)	2.43	511	1.2077	1020	1.59	69
-HC	$S_0 \rightarrow S_2$	H-1→L+1 (13%) H→L (77%)	2.52	493	0.1205	984	7.00	325
	$S_0 \rightarrow S_3$	H-3→L (13%) H-2→L+1 (14%) H-1→L (60%)	2.54	490	0.1328	980	0.27	12.7
	$S_0 \rightarrow S_4$	H-2→L (19%) H-1→L+1 (74%)	2.64	471	0.0681	942	21.3	1080
	$S_0 \rightarrow S_5$	H-3→L (55%) H-2→L+1 (23%)	2.68	462	0.0142	924	4.32	228
	$S_0 \rightarrow S_6$	H-3→L+1 (41%) H-2→L (38%)	2.71	457	0.0048	914	18.7	1000
	$S_1 \rightarrow S_0$	H→L (80%)	2.23	558	0.9913	–	–	–

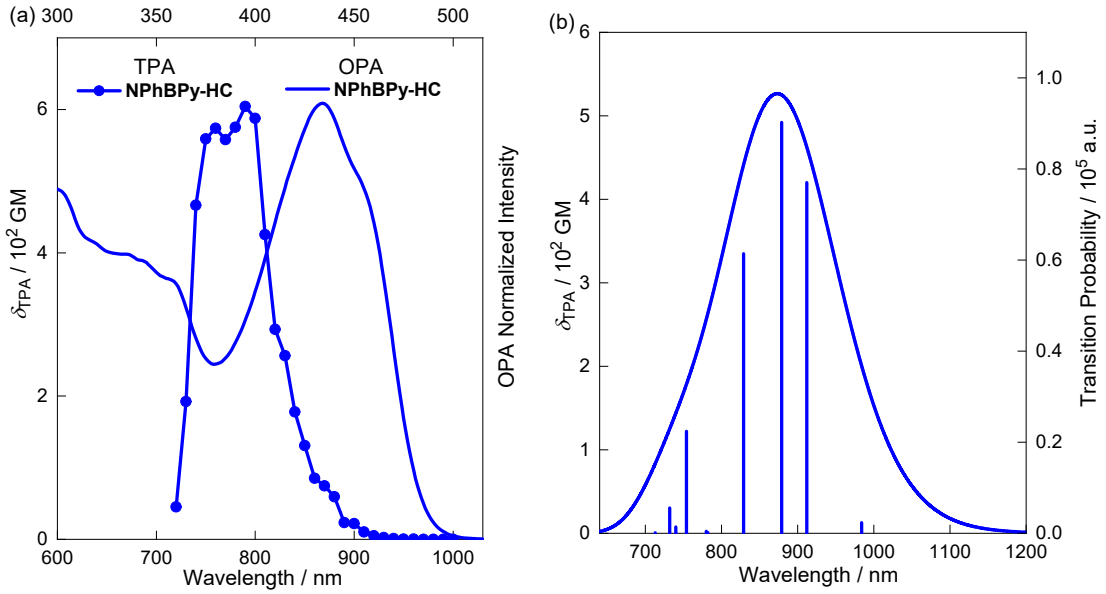


Fig. S12 (a) Rescaled one-photon absorption spectra and two-photon absorption spectra of **NPhBPy-HC** in THF. (b) Calculated TPA spectra from S_0 state to various excited state at the optimized S_0 geometries **NPhBPy-HC**, calculated at TD-B3LYP-D3(BJ)/6-31G(d).

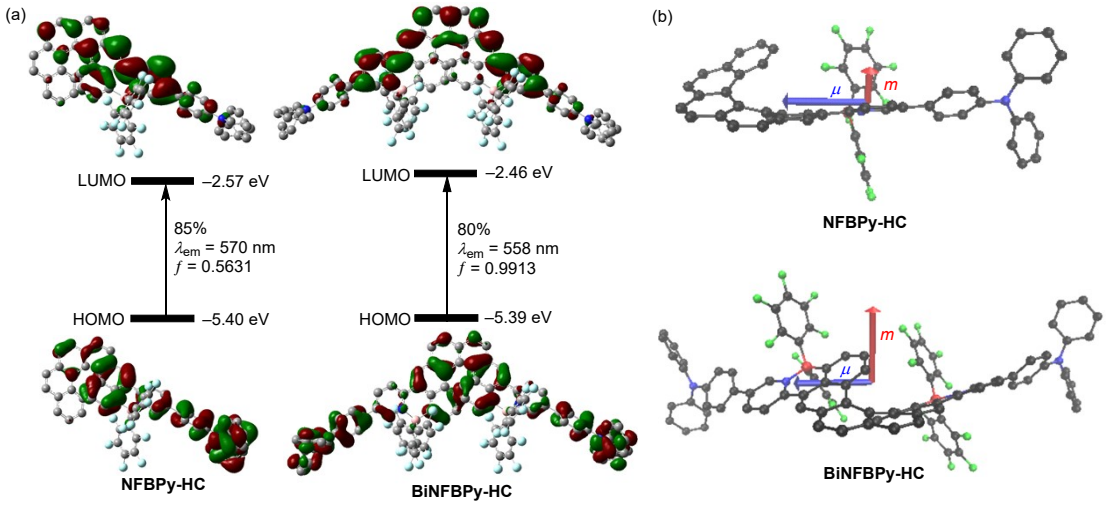


Fig. S13 (a) Kohn–Sham energy levels, pictorial drawing of frontier orbitals, and $S_1 \rightarrow S_0$ transitions, and (b) $S_1 \rightarrow S_0$ transition electronic (blue) and magnetic (red) dipole moments of **NFBPy-HC** and **BiNFBPy-HC**, calculated by TD-DFT at the B3LYP-D3(BJ)/6-31g(d) level for *M*-enantiomers.

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(5) CCDC-2488475 (**PhBPy-HC**), 2488477 (**NFBPy-HC**) contains the supplementary crystallographic data for this paper. These data can be obtained free of charge from The Cambridge Crystallographic Data Centre via www.ccdc.cam.ac.uk/data_request/cif.
(6) J. R. Lakowicz, *Principles of fluorescence spectroscopy*; Springer, 2006; pp 133−143.
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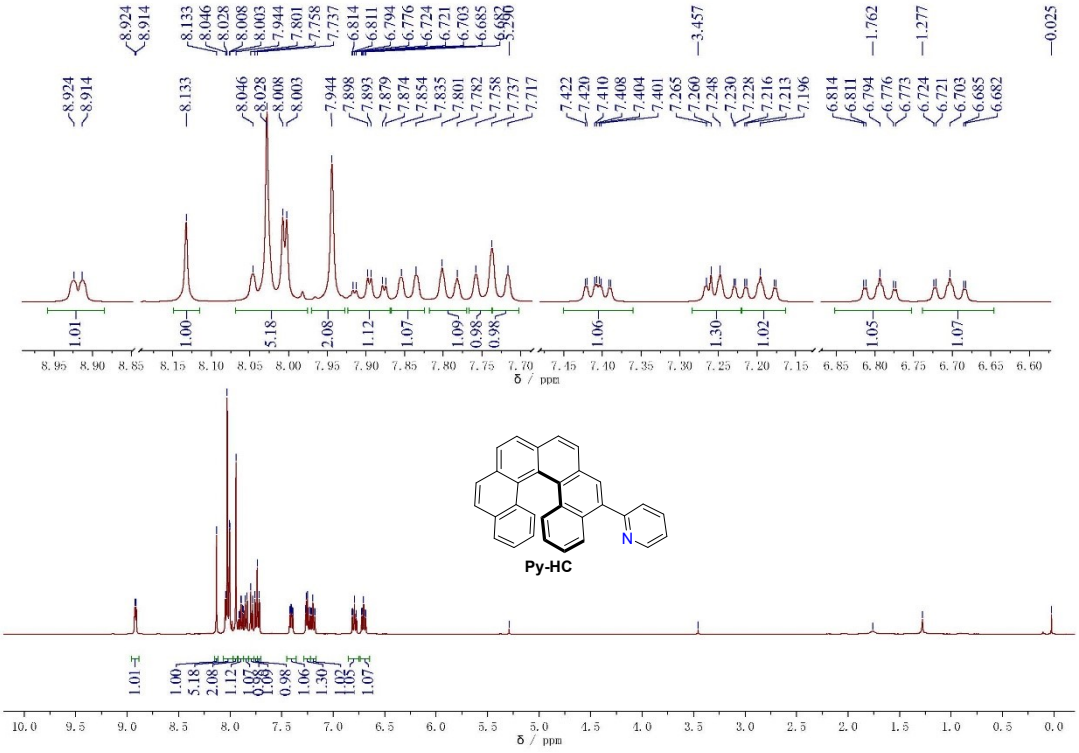
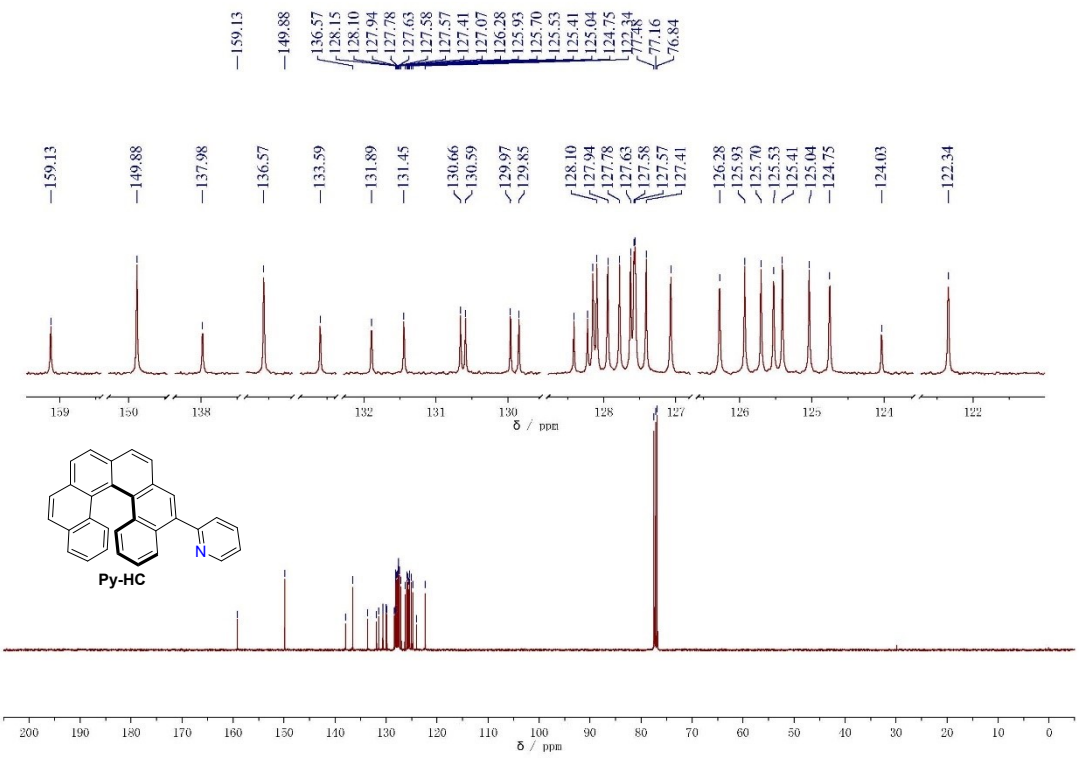
(9) Dalton, a molecular electronic structure program, Release Dalton2021.alpha (2021), see http://daltonprogram.org

NMR and HRMS Spectra

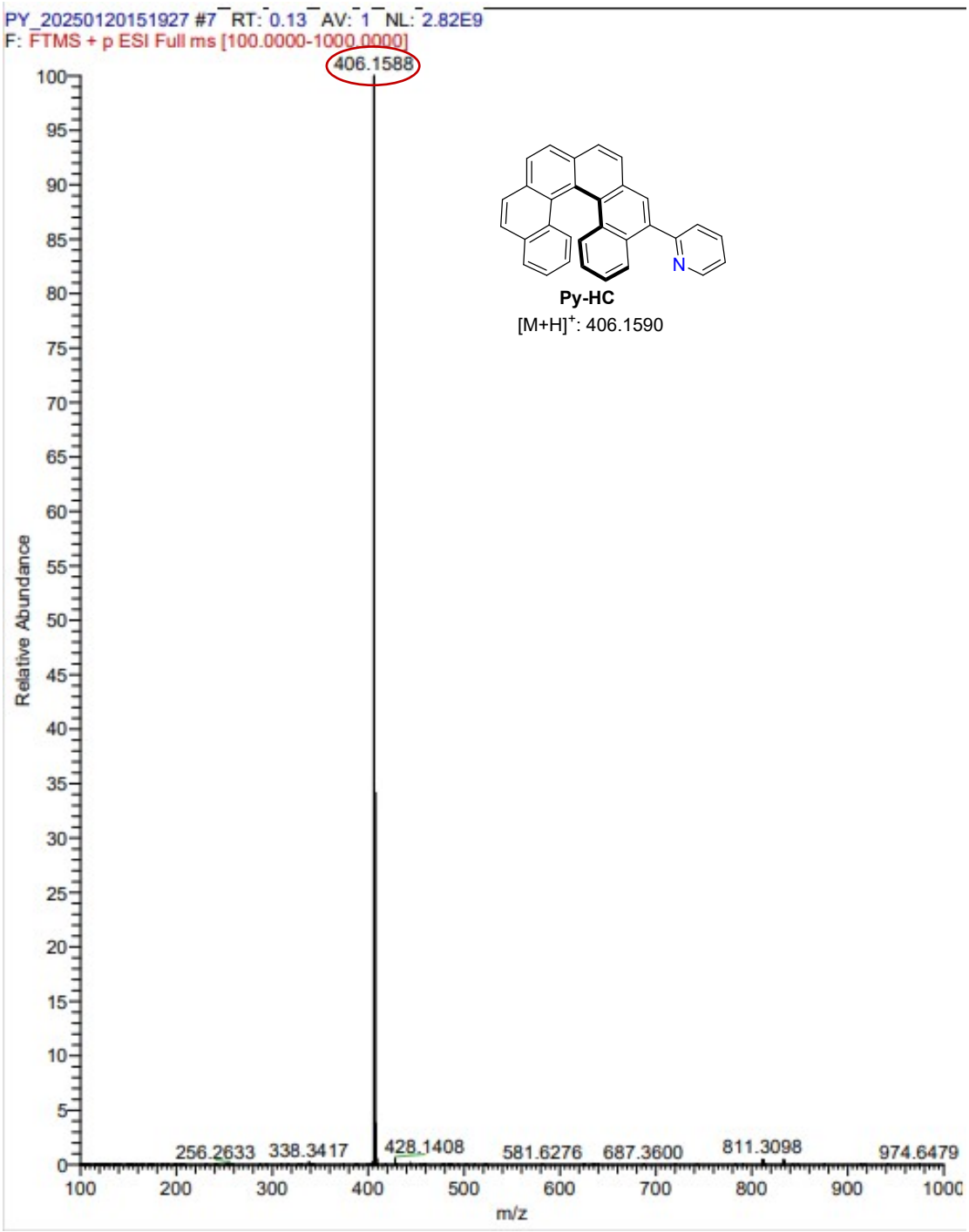
^{1}H NMR of **Py-HC** (400 MHz, $CDCl_3$, rt)



^{13}C{^{1}H} NMR of **Py-HC** (100 MHz, $CDCl_3$, rt)



HRMS of **Py-HC**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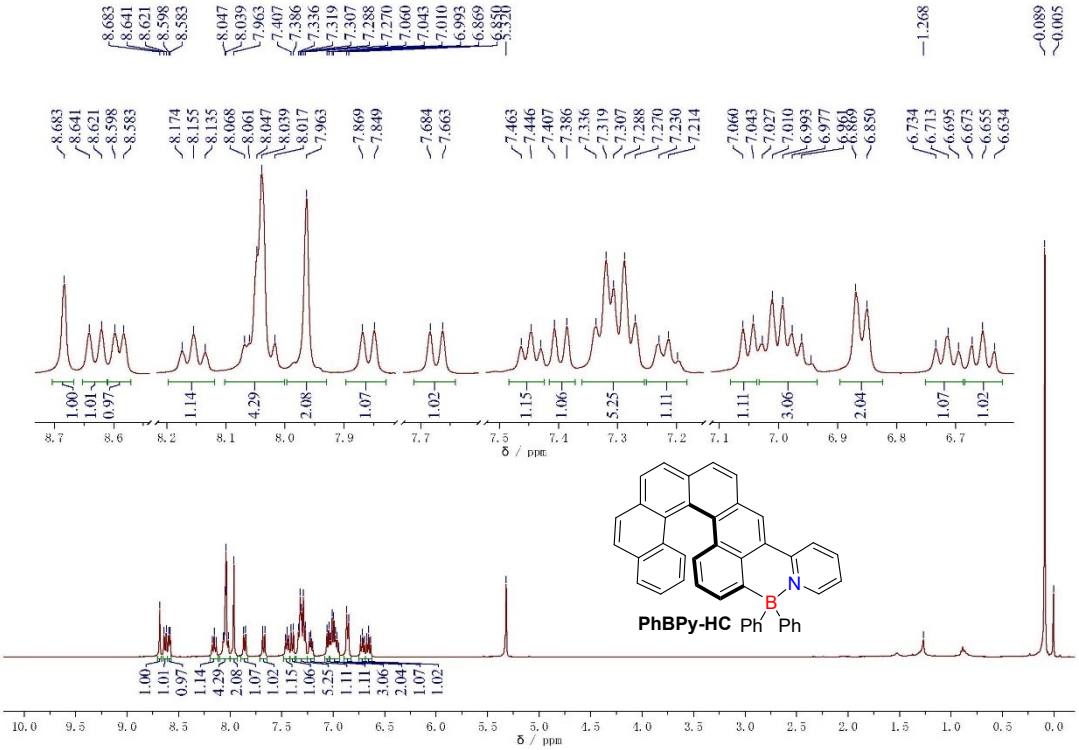
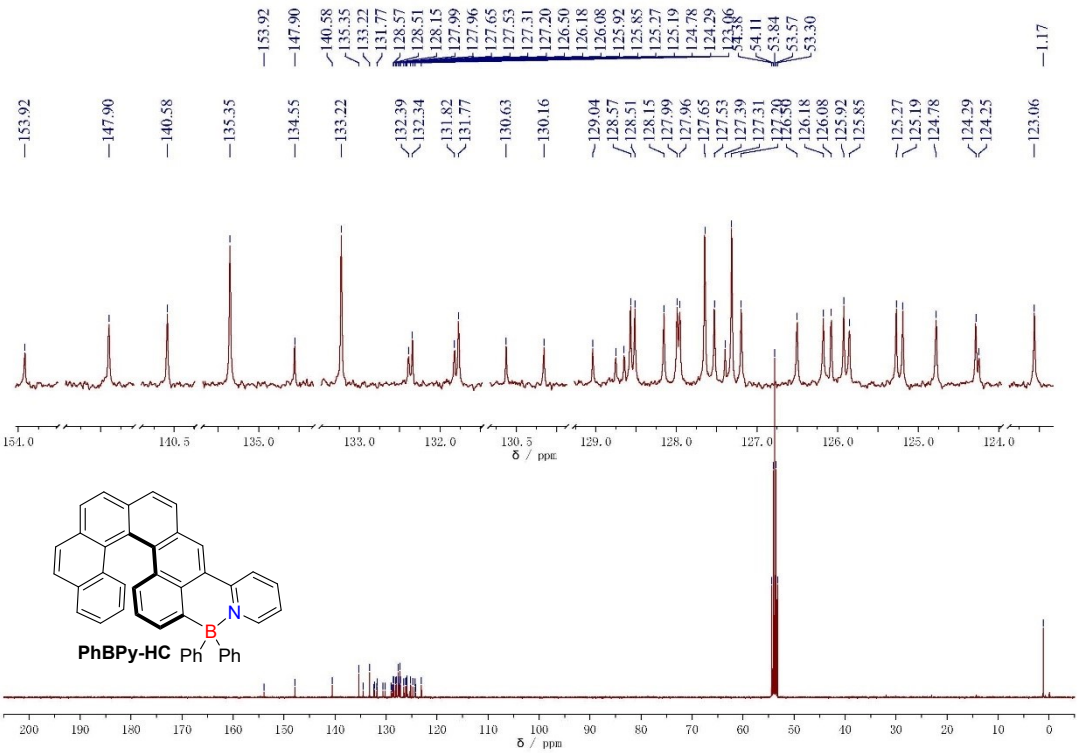
406.1588
N
Py-HC
[M+H]+: 406.1590
Relative Abundance
m/z
256.2633
338.3417
428.1408
581.6276
687.3600
811.3098
974.6479

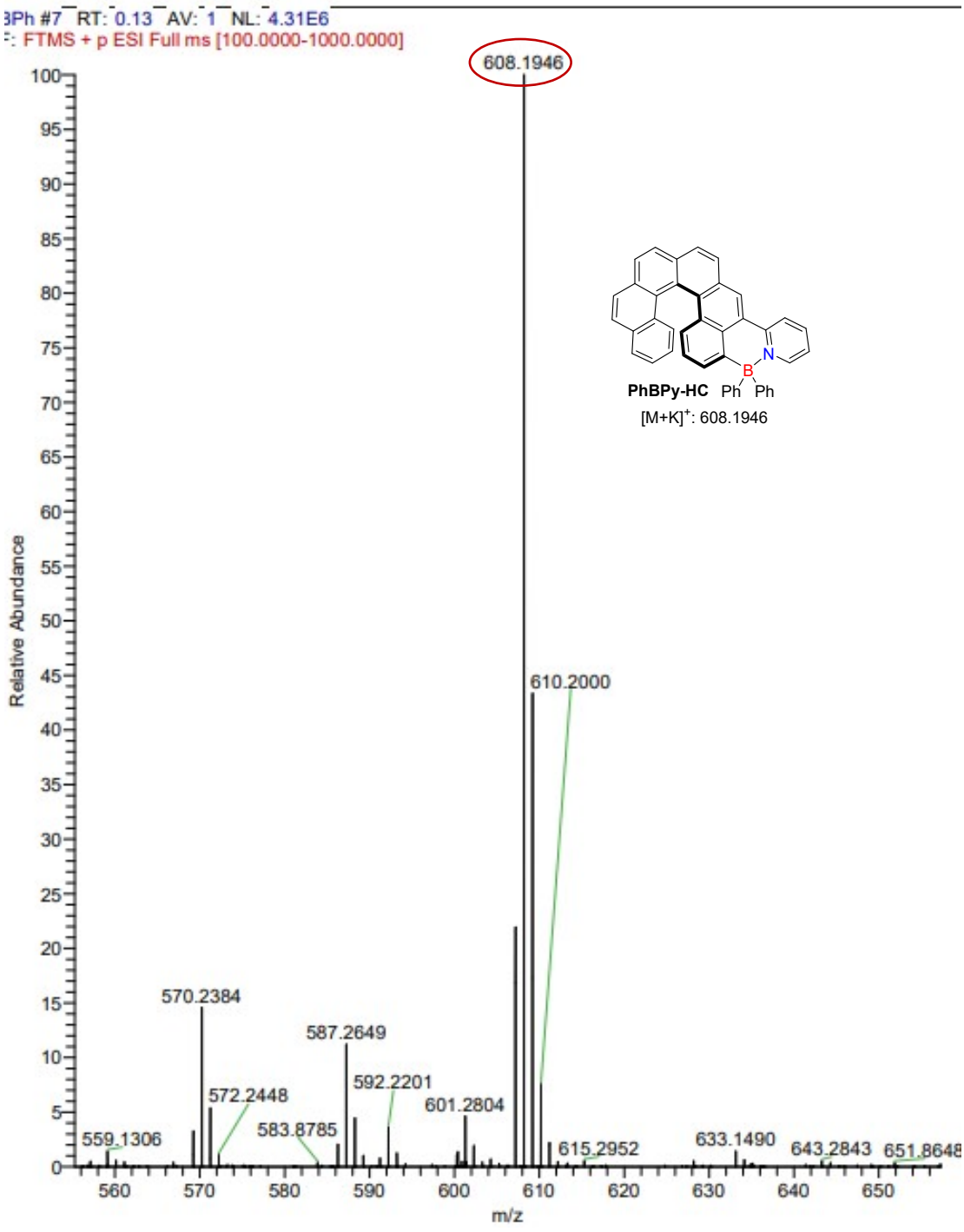
^{1}H NMR of **PhBPy-HC** (400 MHz, CD_2Cl_2, rt)



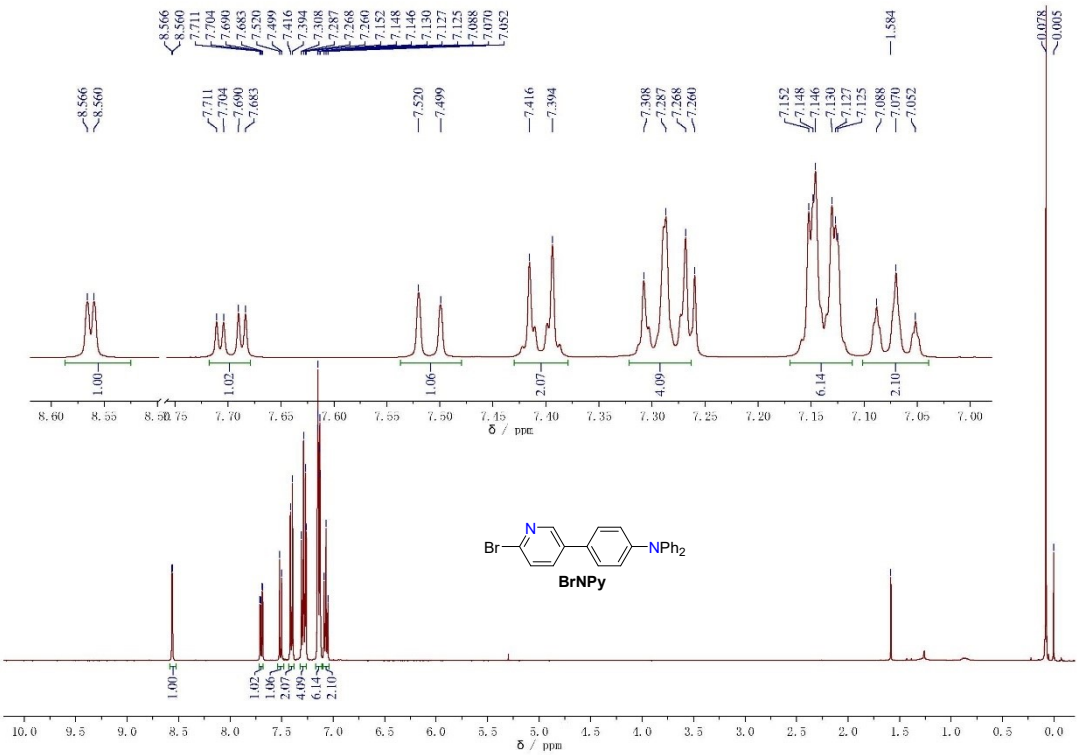
^{13}C{^{1}H} NMR of **PhBPy-HC** (100 MHz, CD_2Cl_2, rt)



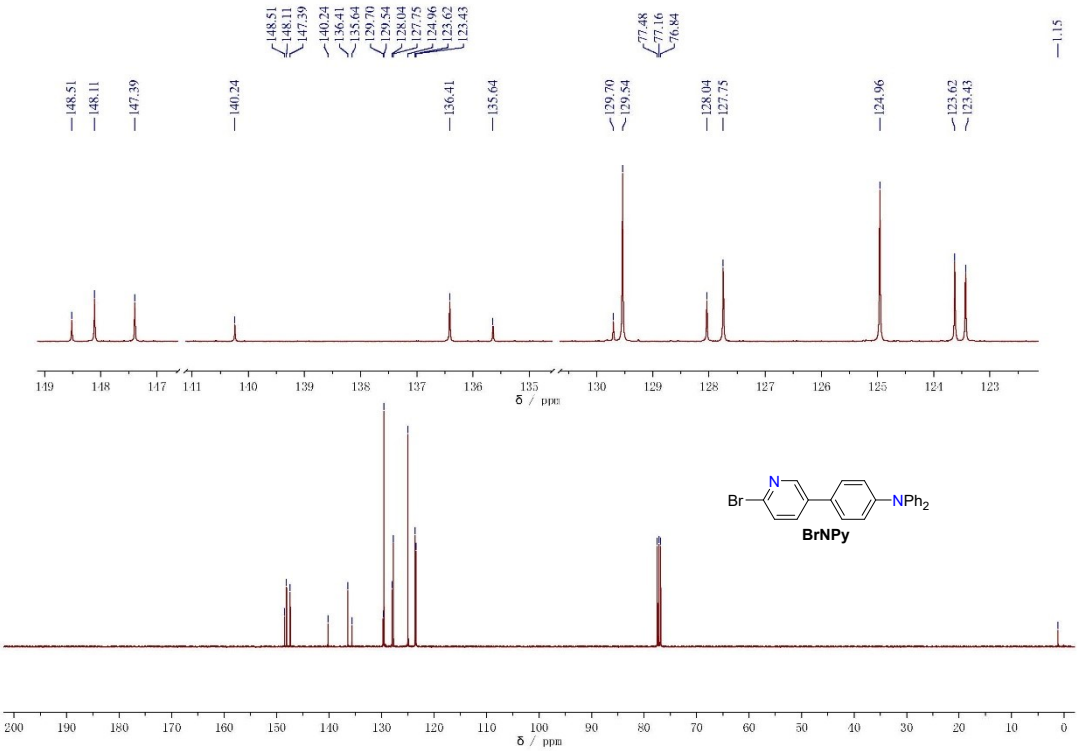
HRMS of **PhBPy-HC**



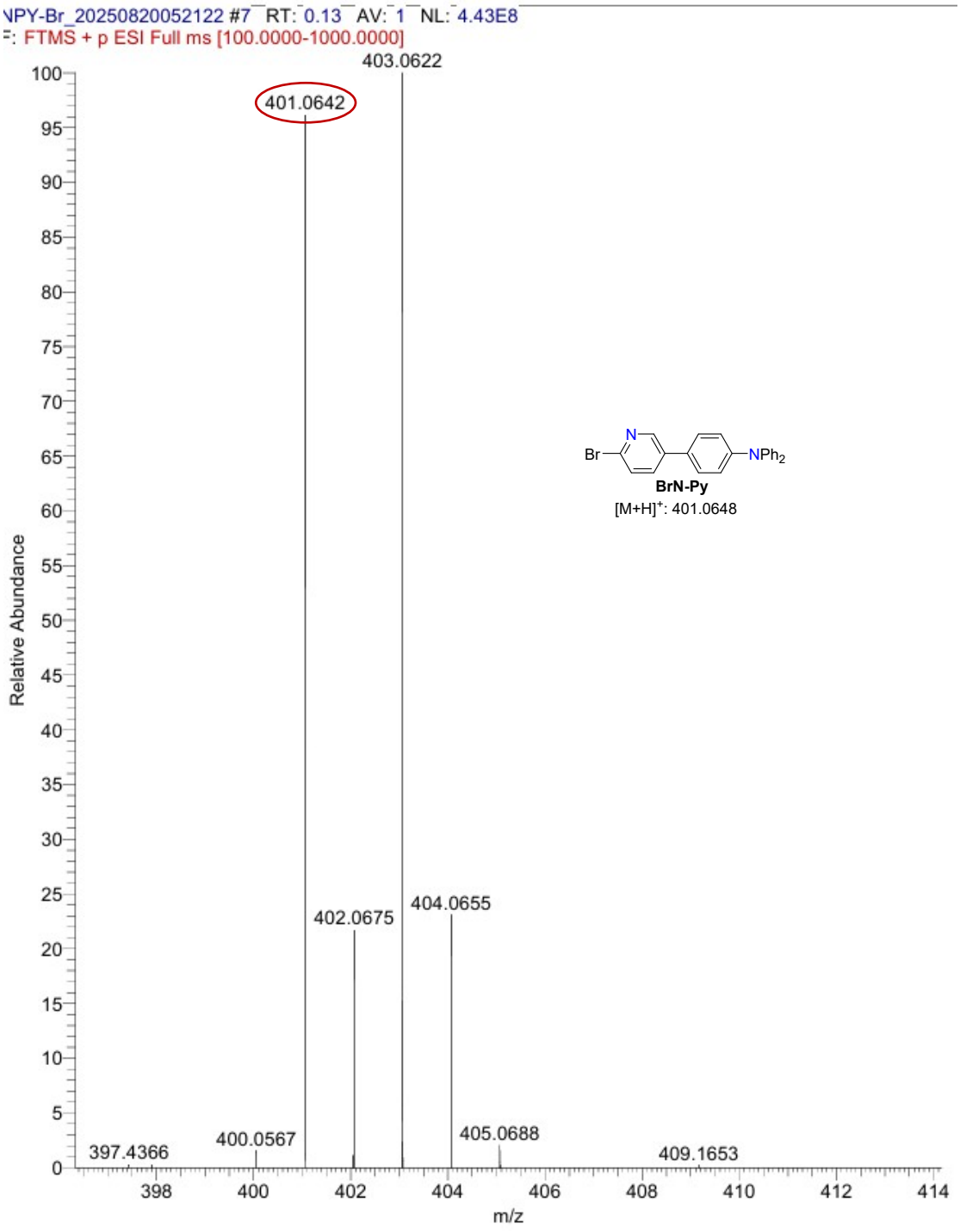
^{1}H NMR of **BrNPy** (400 MHz, $CDCl_3$, rt)



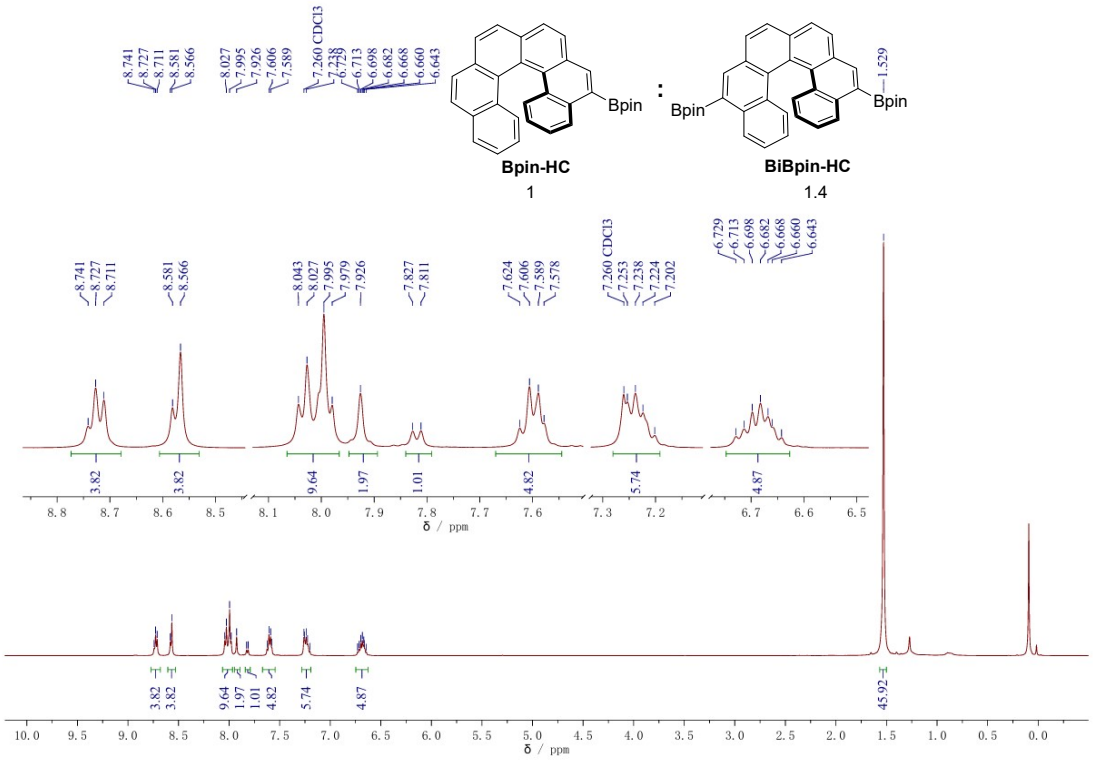
^{13}C{^{1}H} NMR of **BrNPy** (100 MHz, $CDCl_3$, rt)



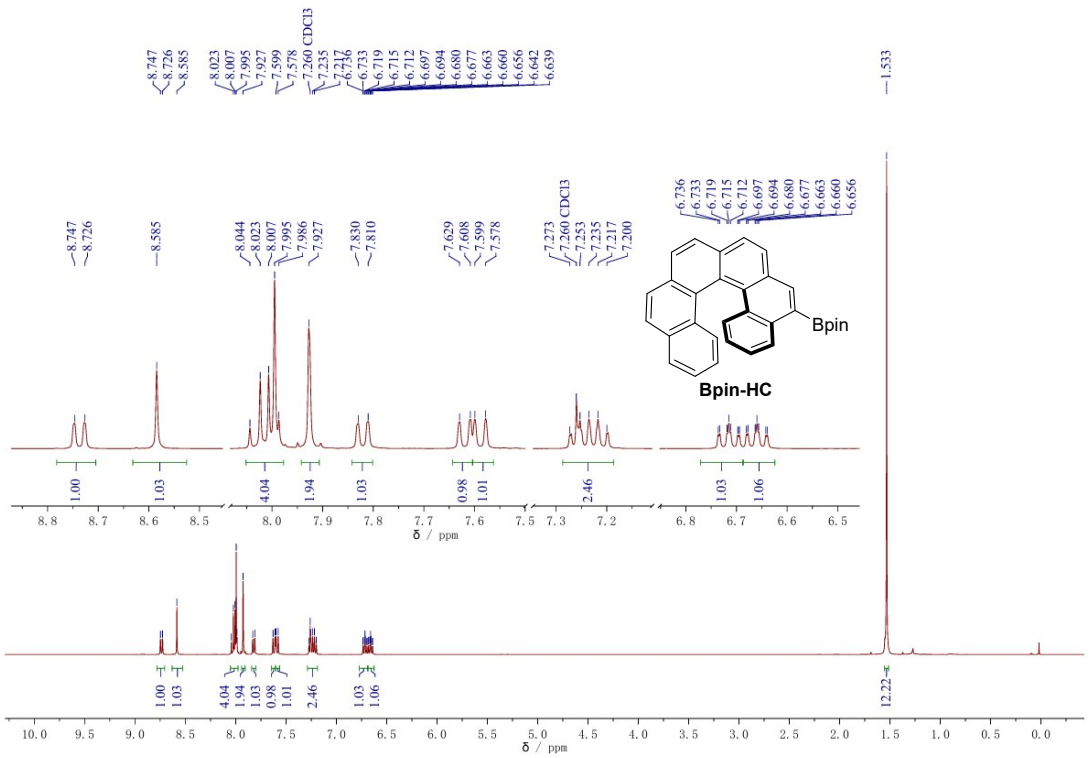
HRMS of **BrNPy**



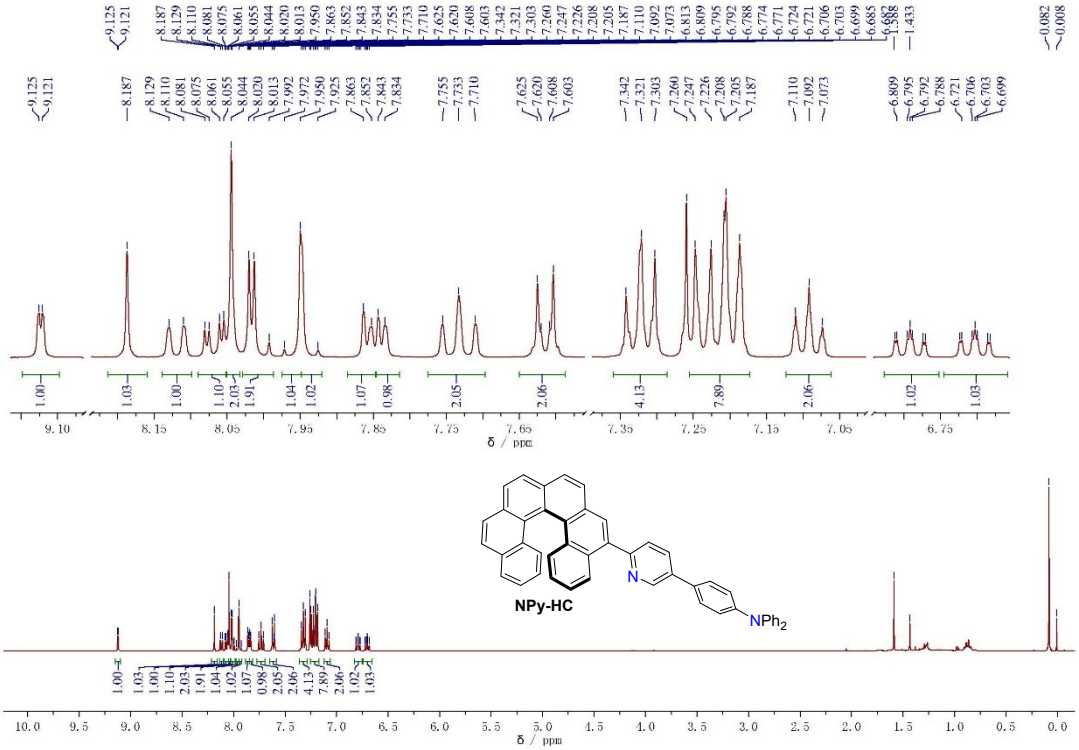
^{1}H NMR of the mixture of **Bpin-HC** and **BiBpin-HC** (500 MHz, $CDCl_3$, rt)



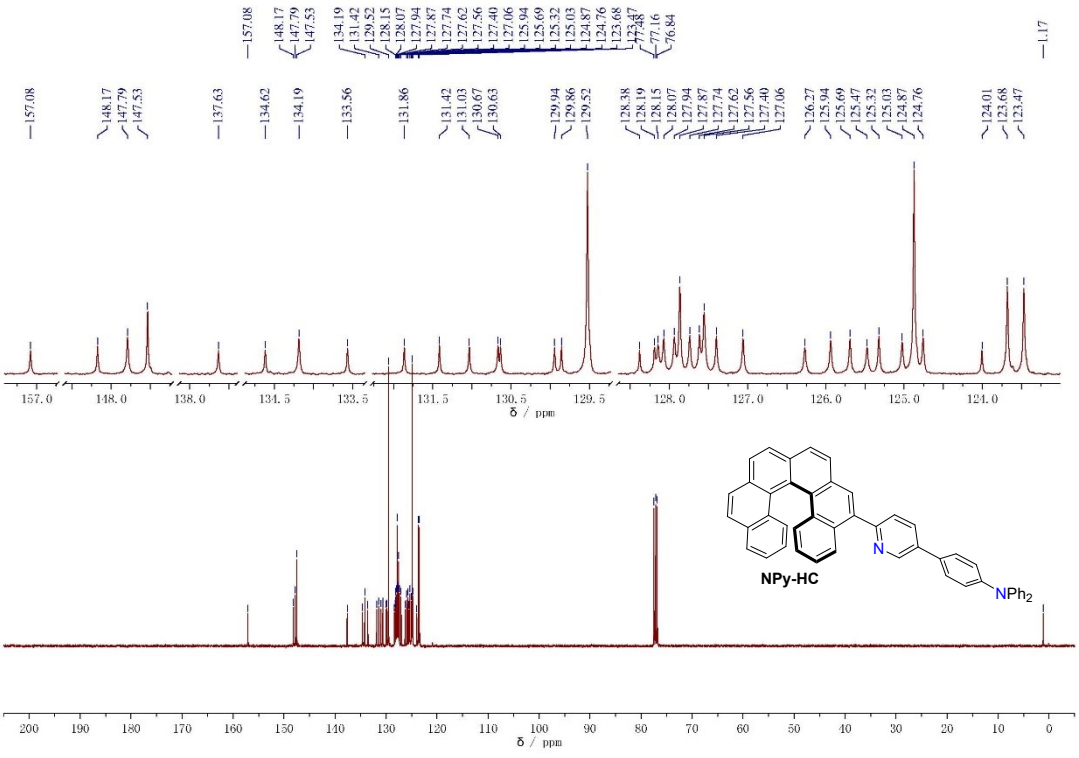
^{1}H NMR of **Bpin-HC** (400 MHz, $CDCl_3$, rt)



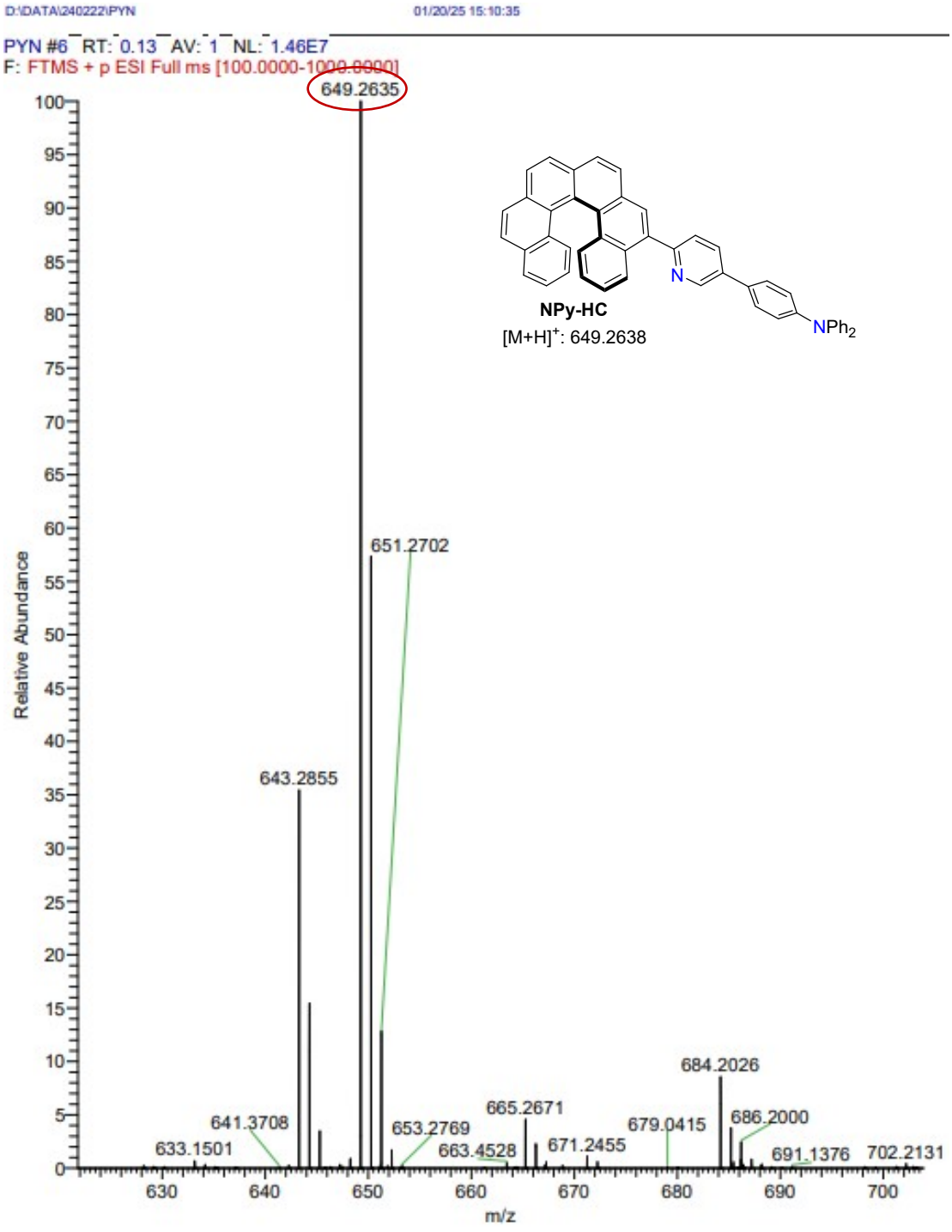
^{1}H NMR of **NPy-HC** (400 MHz, $CDCl_3$, rt)



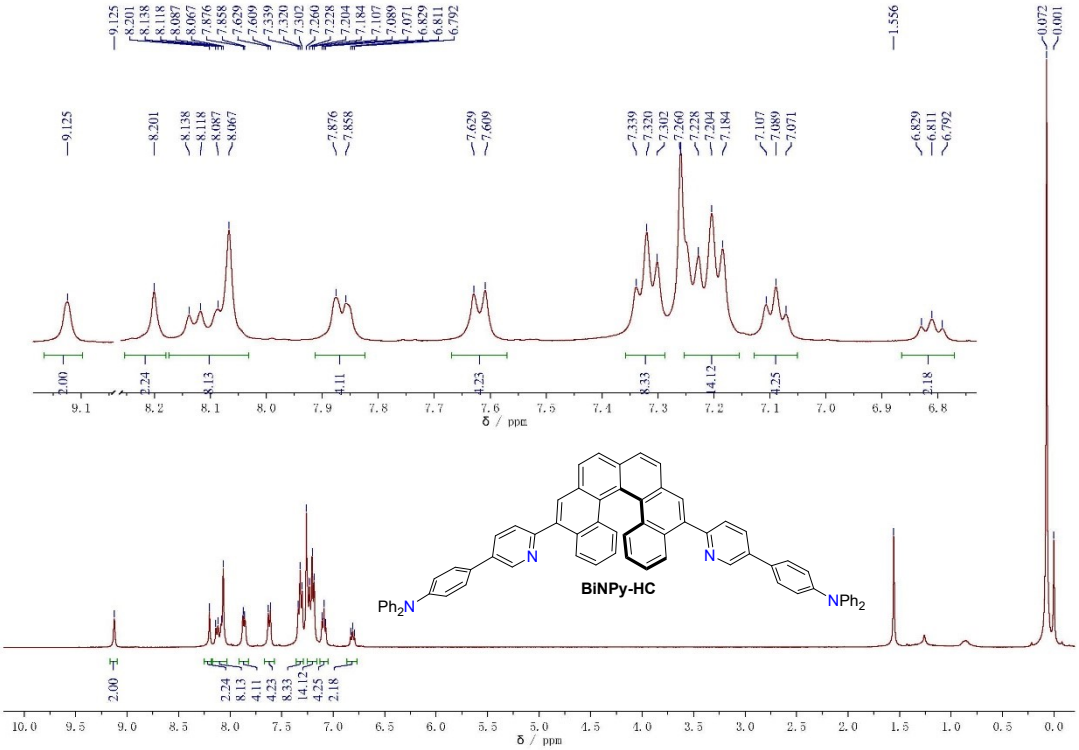
^{13}C{^{1}H} NMR of **NPy-HC** (100 MHz, $CDCl_3$, rt)



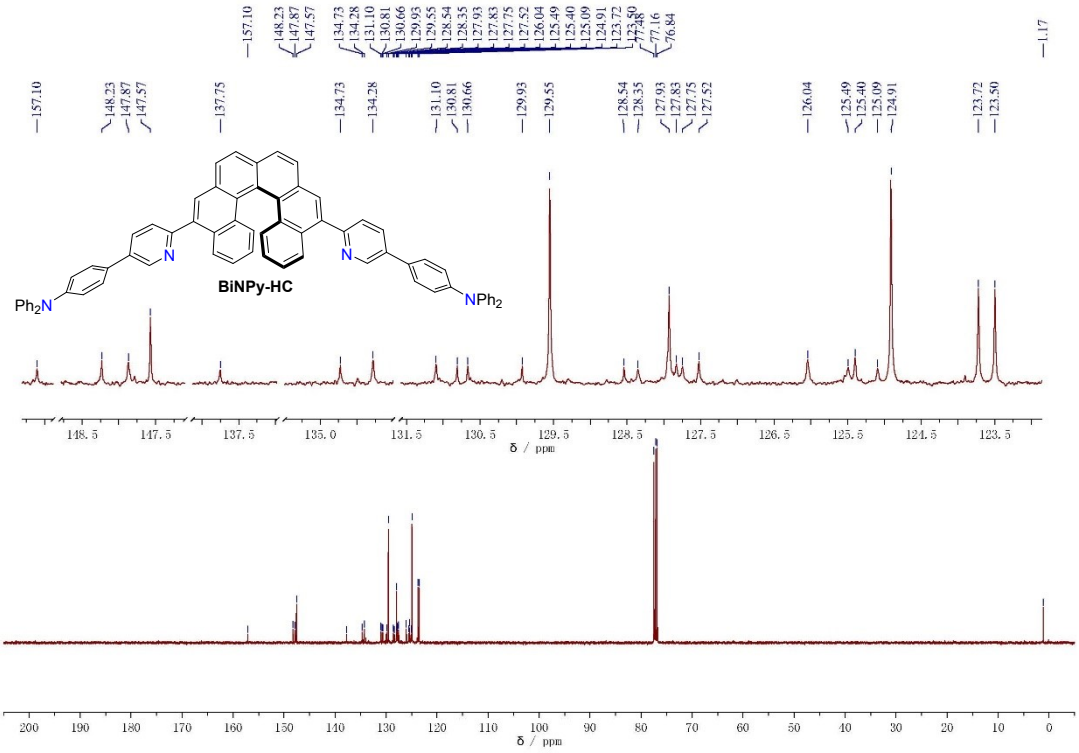
HRMS of **NPy-HC**



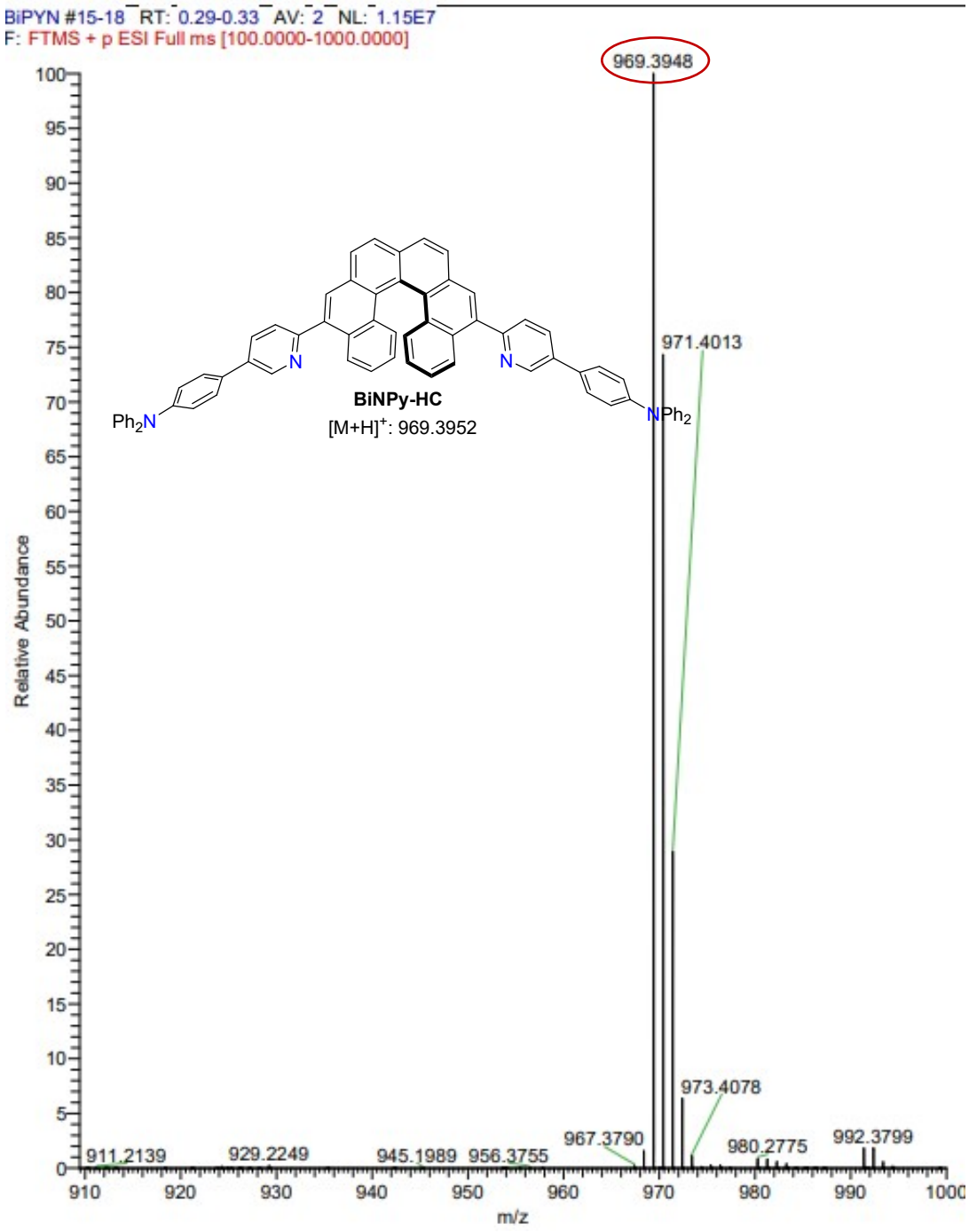
^{1}H NMR of **BiNPy-HC** (400 MHz, $CDCl_3$, rt)



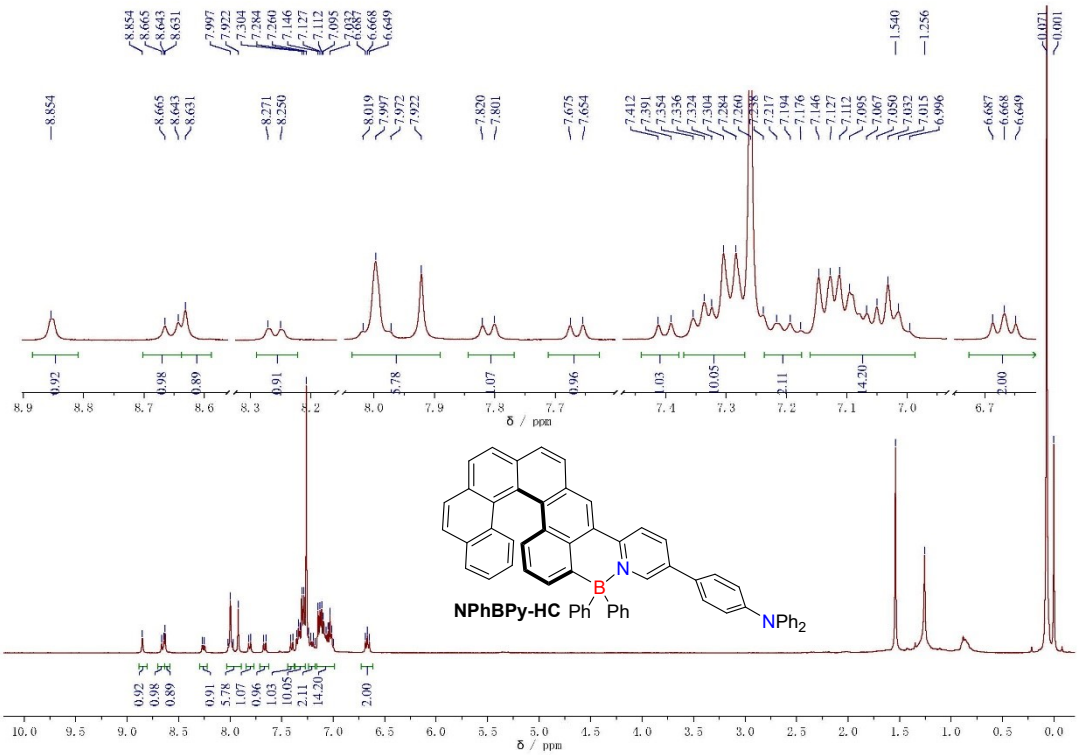
^{13}C{^{1}H} NMR of **BiNPy-HC** (100 MHz, $CDCl_3$, rt)



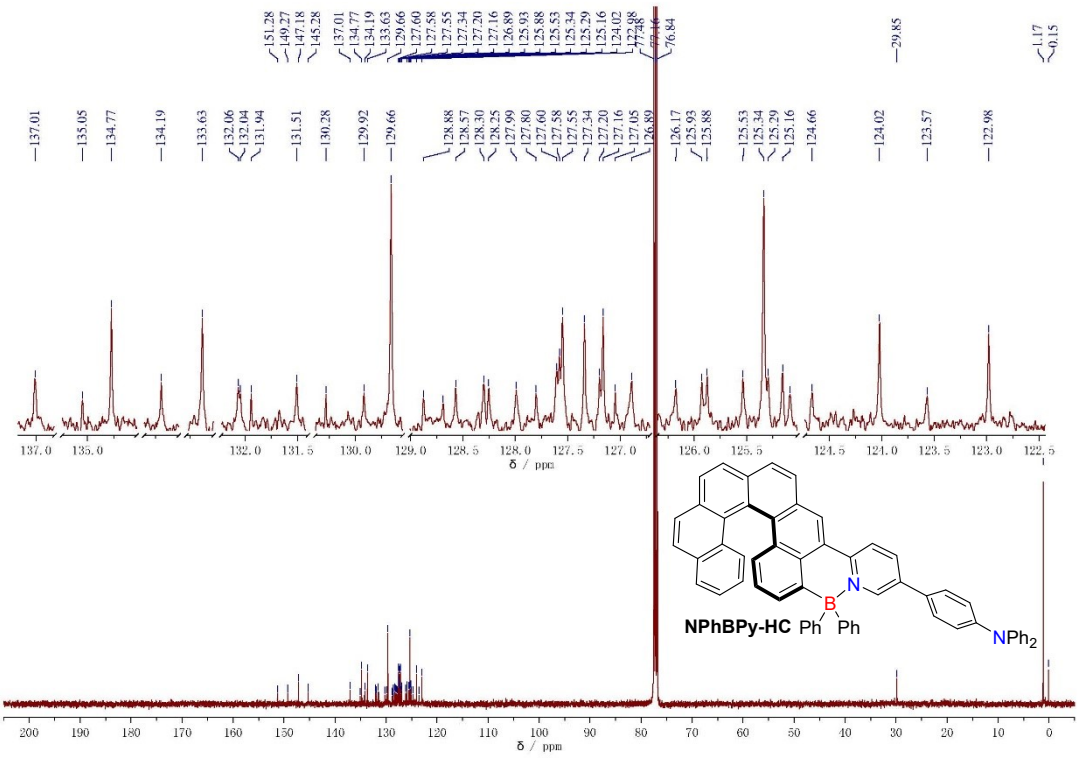
HRMS of **BiNPy-HC**



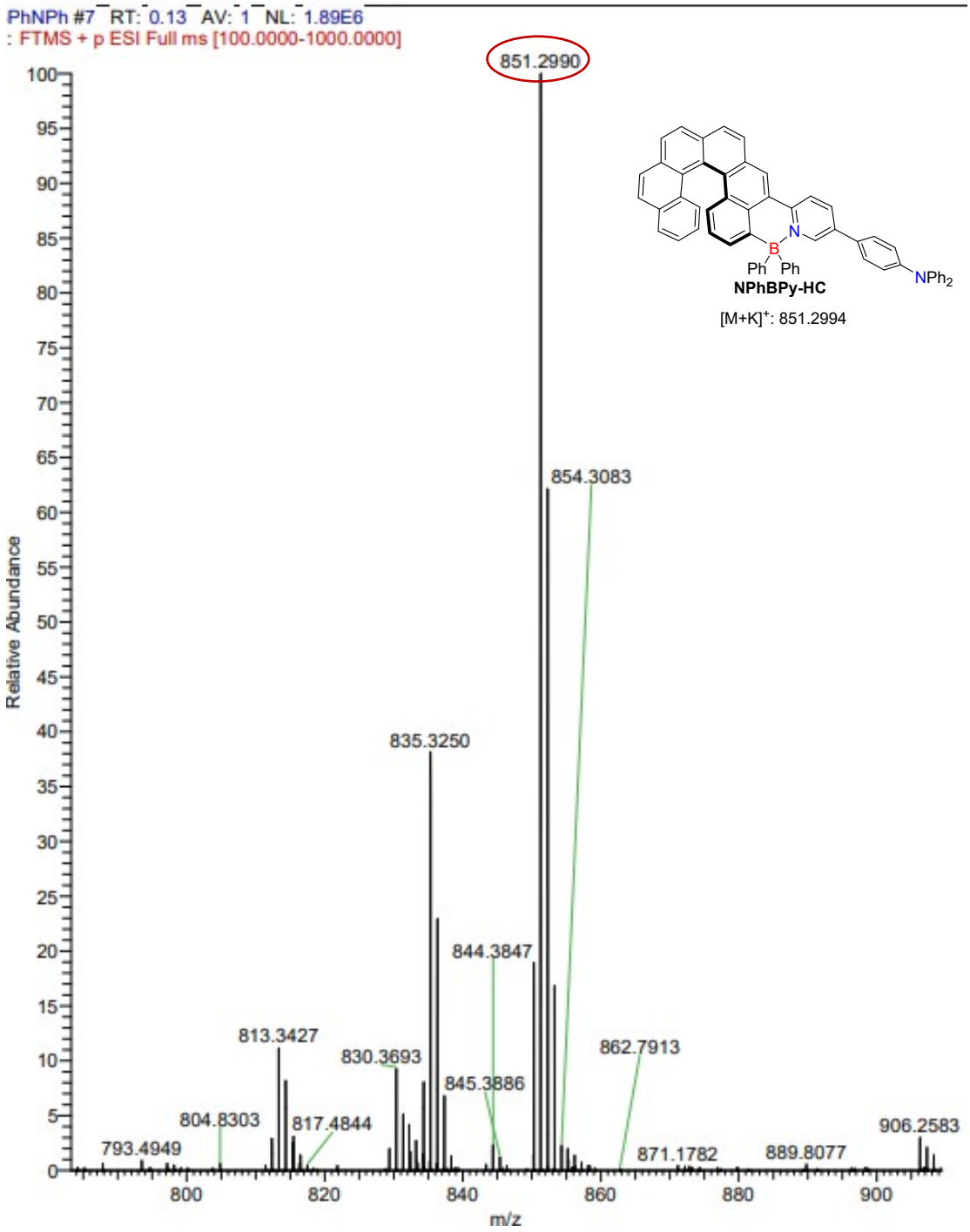
^{1}H NMR of **NPhBPy-HC** (400 MHz, $CDCl_3$, rt)



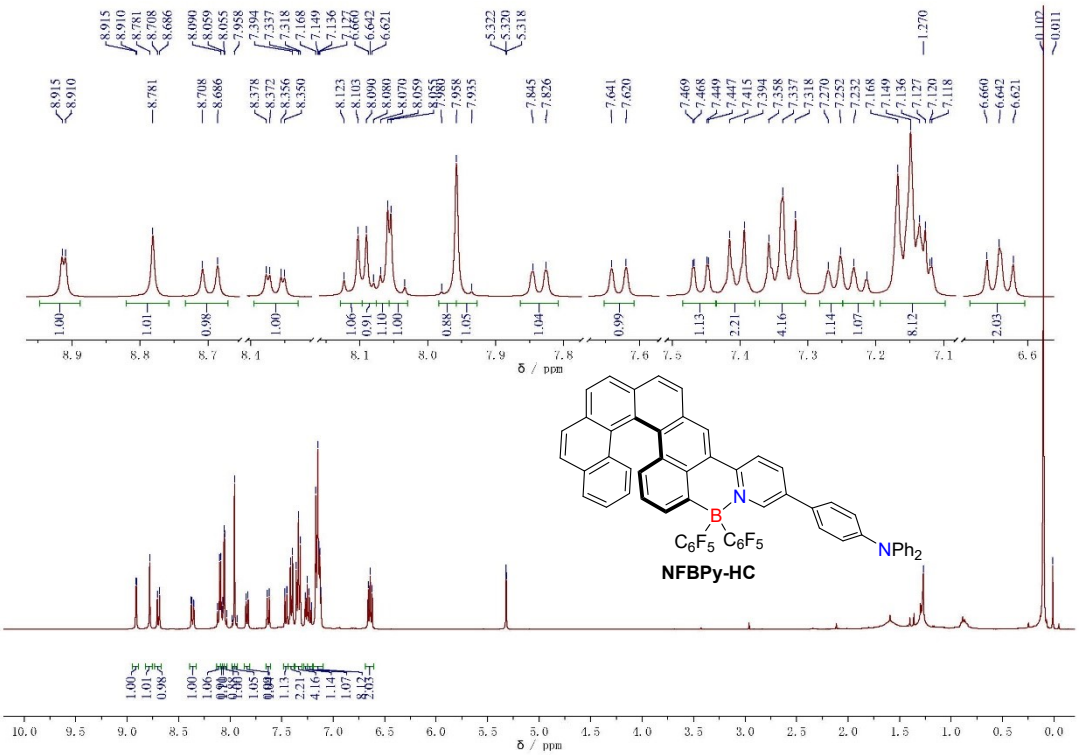
^{13}C{^{1}H} NMR of **NPhBPy-HC** (100 MHz, $CDCl_3$, rt)



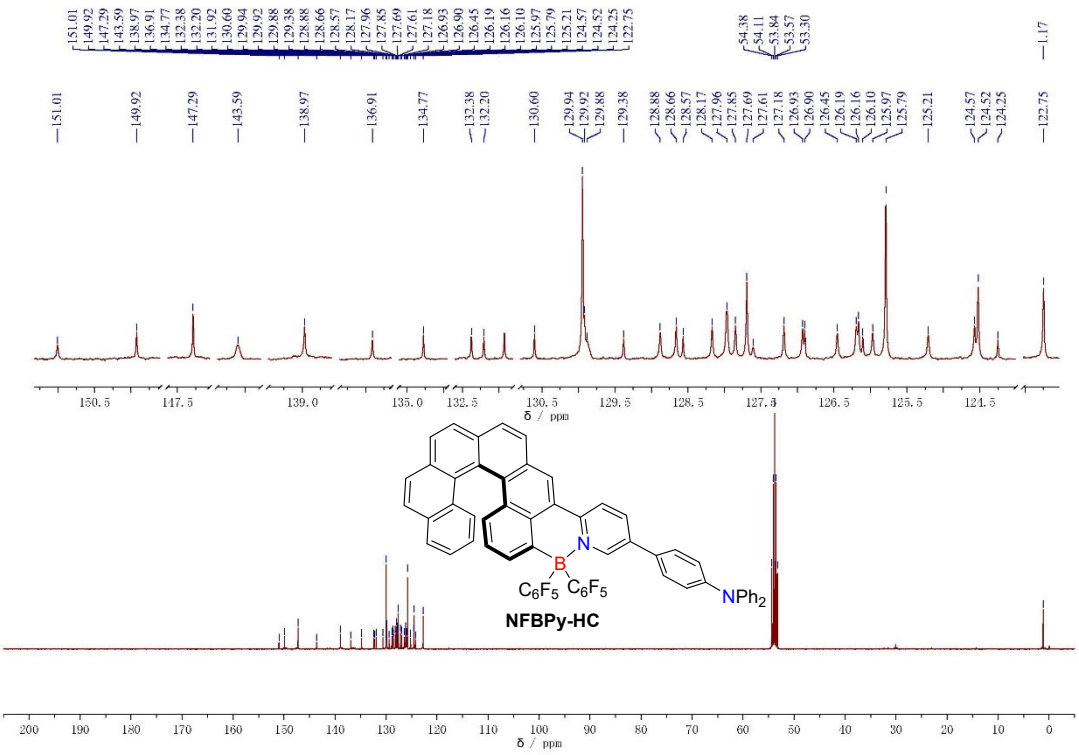
HRMS of **NPhBPy-HC**



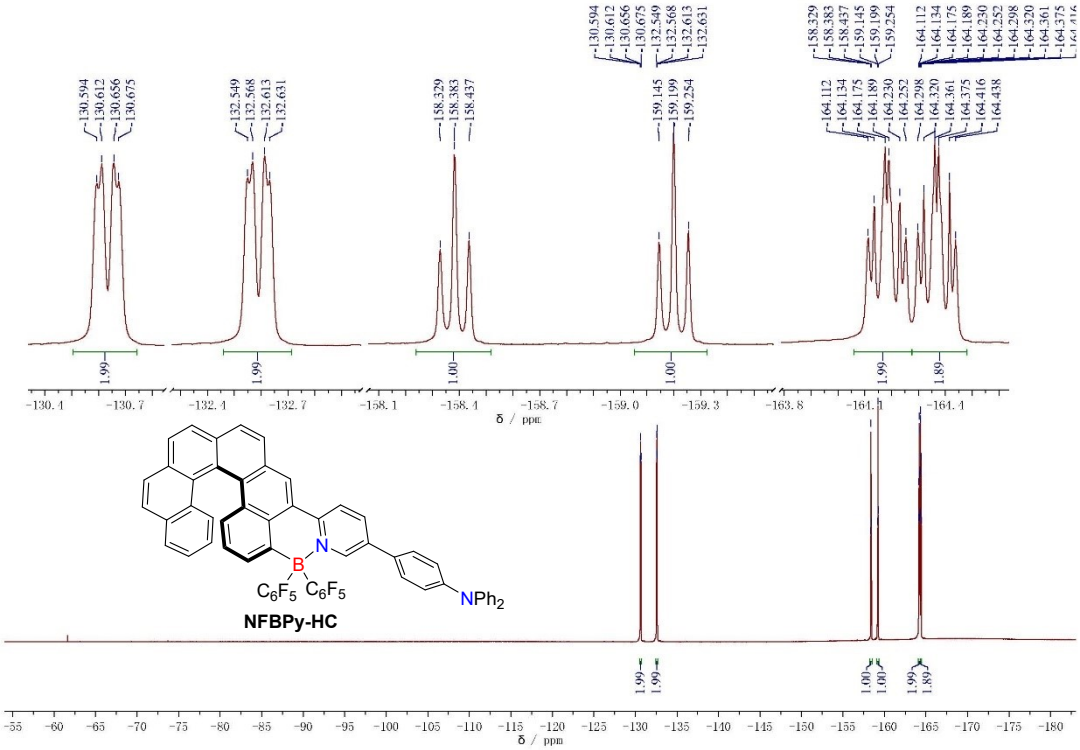
^{1}H NMR of **NFBPy-HC** (400 MHz, CD_2Cl_2, rt)



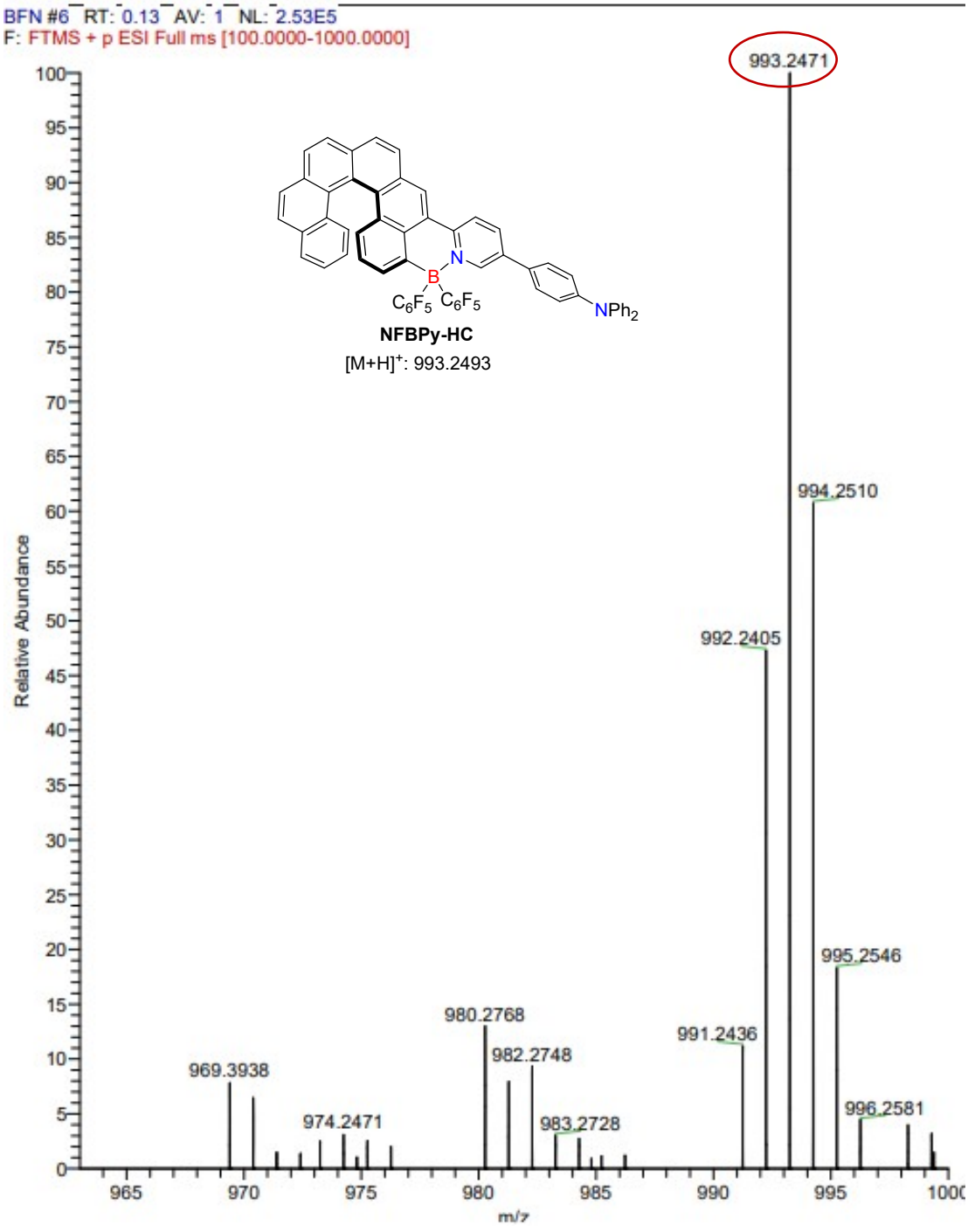
^{13}C{^{1}H} NMR of **NFBPy-HC** (100 MHz, CD_2Cl_2, rt)



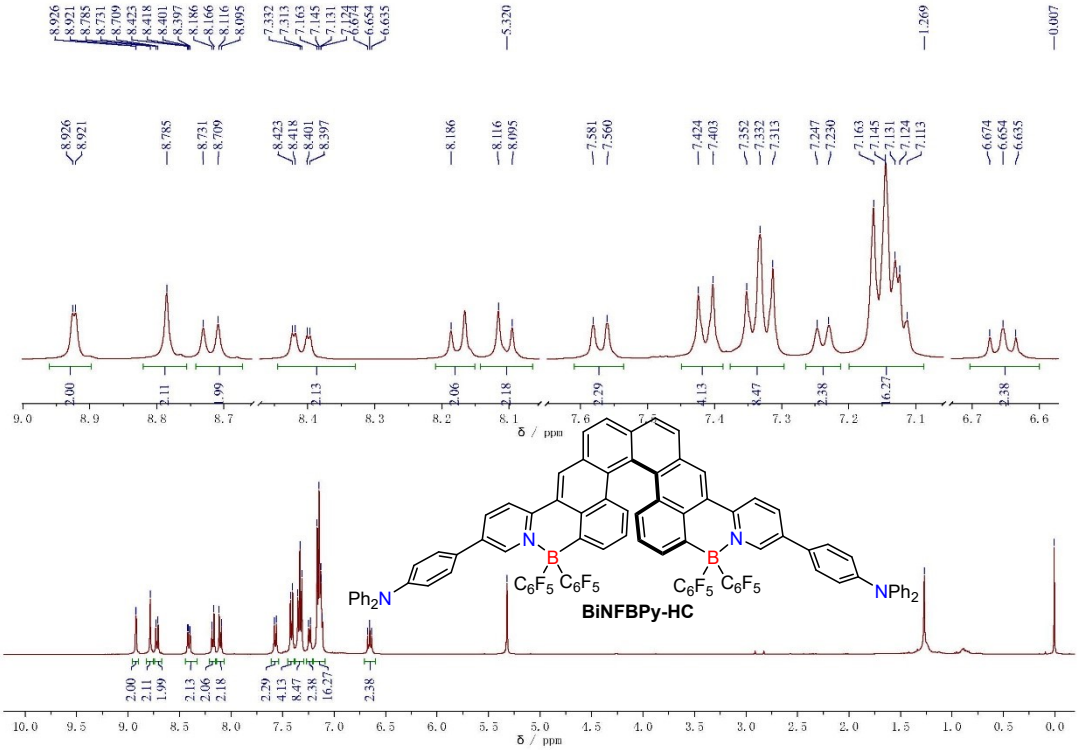
^{19}F NMR of **NFBPy-HC** (367 MHZ, $CDCl_3$, r.t.)



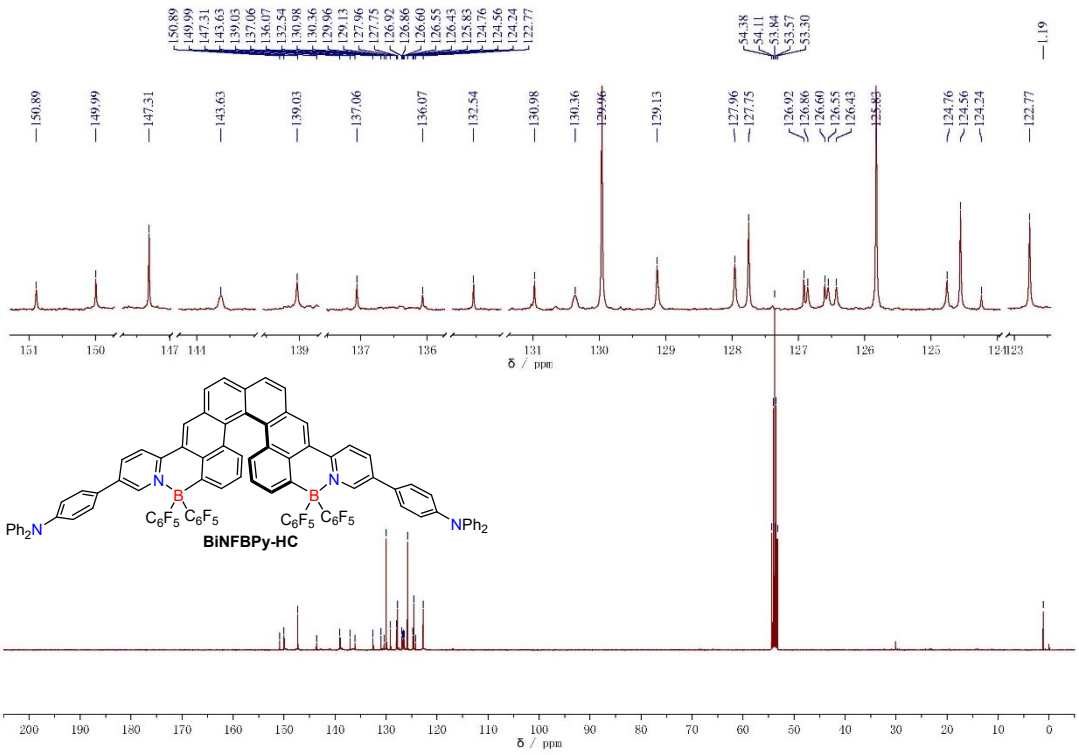
HRMS of **NFBPy-HC**



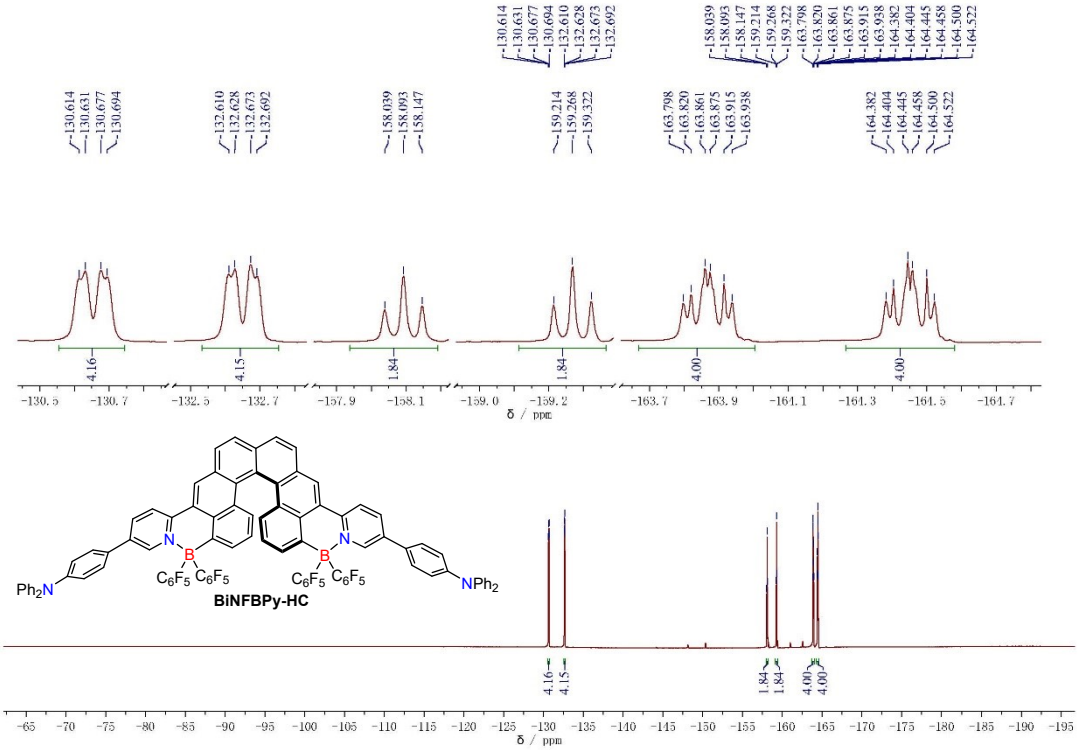
^{1}H NMR of **BiNFBPy-HC** (400 MHz, CD_2Cl_2, rt)



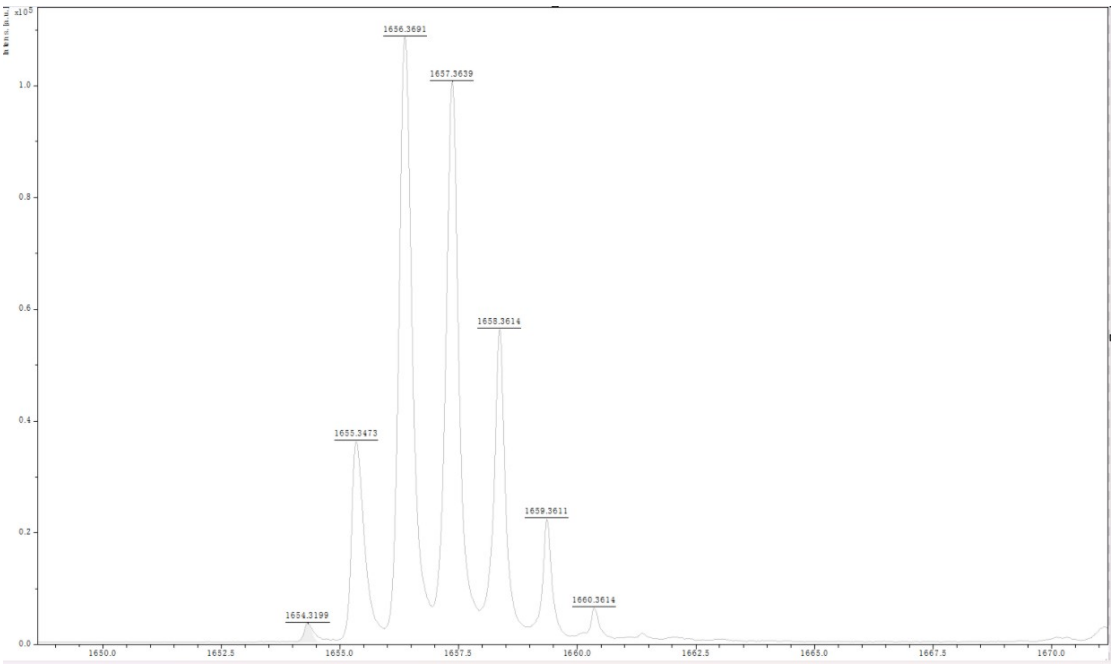
^{13}C{^{1}H} NMR of **BiNFBPy-HC** (100 MHz, CD_2Cl_2, rt)



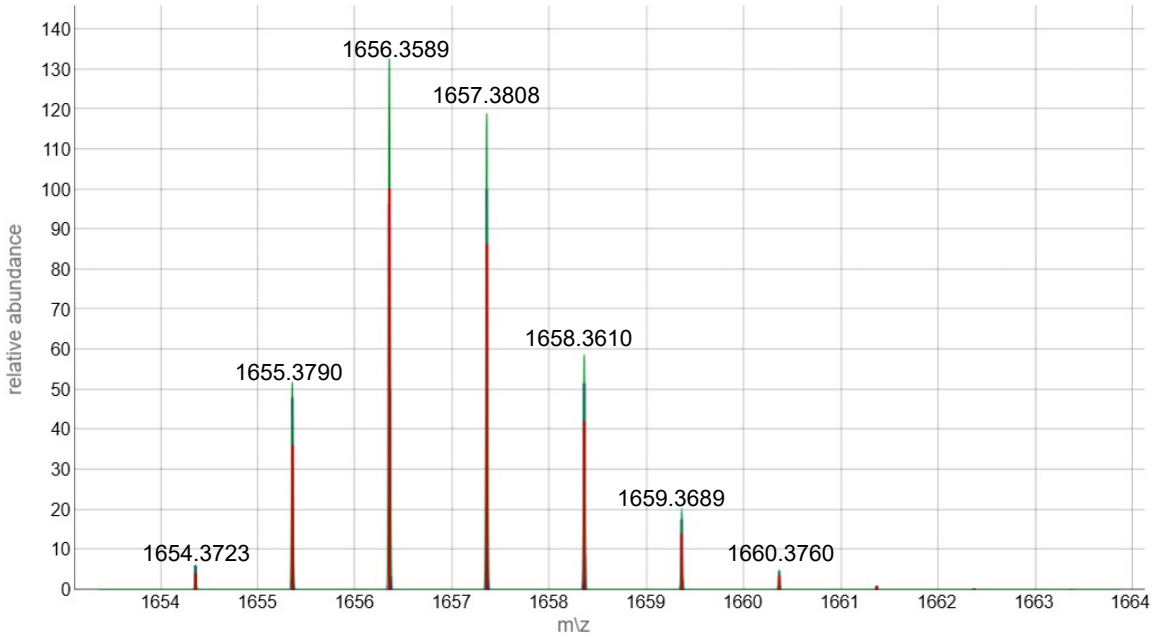
^{19}F NMR of **BiNFBPy-HC** (367 MHZ, $CDCl_3$, r.t.)



MS(MALDI-TOF) of **BiNFBPy-HC**



Simulation of ESI-MS $[M]^{\bullet+}$ for **BiNFBPy-HC**



Total Energies and Cartesian Coordinates of Optimized Structures

Compound (*M*)-**PhBPy-HC** in S_0 state**.**

Total energy (PBE0-D3(BJ)/6-31G(d)) −1733.226115 a. u.

	X	Y	Z
N	-2.87610400	-0.48965900	-1.25672300
C	-4.02339600	-0.35209400	-1.94300800
H	-4.74602200	0.31707100	-1.49125000
C	-4.26817900	-1.01404500	-3.12841000
H	-5.21303000	-0.87064300	-3.63998800
C	-3.27066100	-1.84235700	-3.63624700
H	-3.40828200	-2.36699200	-4.57714700
C	-2.08600800	-1.97080200	-2.93635100
H	-1.27667700	-2.56579200	-3.34023800
C	-1.89602700	-1.30339900	-1.71725200
C	-0.62859000	-1.40840500	-0.99086600
C	0.22570900	-2.45312100	-1.23636900
H	-0.09953300	-3.31844100	-1.80759100
C	1.56682500	-2.44700800	-0.77492400
C	2.09042000	-1.28365100	-0.16225500
C	1.13348200	-0.32749600	0.35633500
C	-0.22737200	-0.38865600	-0.05947900
C	-1.20441100	0.49219800	0.46034300
C	-0.78952000	1.45866600	1.36252000
H	-1.51879300	2.16295500	1.75588800
C	0.53528900	1.50859300	1.81865400
H	0.82214300	2.23631900	2.57330700
C	1.47387300	0.62206600	1.34161200
H	2.48092500	0.64127200	1.73932000
C	2.38048400	-3.60132100	-0.93789000
H	1.94444000	-4.48964200	-1.38782200
C	3.65185700	-3.61105000	-0.45225600
H	4.25026500	-4.51819600	-0.46812500
C	4.24788800	-2.41497900	0.03368000

C	3.52073100	-1.19244100	0.00971900
C	4.27056500	0.03290500	0.16930000
C	5.54115600	-0.03967300	0.78698100
C	6.16055300	-1.30042800	0.99933800
H	7.14470300	-1.32552200	1.46020100
C	5.57230600	-2.44186400	0.54461600
H	6.08758300	-3.39723300	0.60122500
C	6.22736100	1.15496200	1.16026000
H	7.16774200	1.05917400	1.69728700
C	5.71942600	2.37838700	0.86075000
H	6.23074200	3.28605500	1.17137600
C	4.54959600	2.49343900	0.05337400
C	3.85191300	1.32034300	-0.35022800
C	2.82352900	1.47023600	-1.30706900
H	2.33791300	0.58854400	-1.70628000
C	2.43760200	2.71131000	-1.76050000
H	1.64308100	2.78880200	-2.49720100
C	3.06636500	3.87301000	-1.28150600
H	2.74473800	4.85092100	-1.62830500
C	4.11695800	3.75796000	-0.40156200
H	4.65068700	4.64153500	-0.05956500
C	-3.64347000	1.56418400	0.17523400
C	-4.85526500	1.70010900	0.86467900
H	-5.21436200	0.86776800	1.46573000
C	-5.60479100	2.87484600	0.80502300
H	-6.53948000	2.94988900	1.35601100
C	-5.15686400	3.95055400	0.04497500
H	-5.73753900	4.86847000	-0.00285100
C	-3.95334000	3.84387500	-0.65018300
H	-3.59068900	4.68146800	-1.24178300
C	-3.21334800	2.66818600	-0.57934900
H	-2.26697300	2.60254500	-1.11436400
C	-3.30424300	-0.90212900	1.25884200
C	-3.97173900	-2.08013600	0.90298000
H	-4.13576700	-2.31920800	-0.14637900

C	-4.44304400	-2.98048900	1.85836300
H	-4.95393600	-3.88687400	1.54106200
C	-4.26005600	-2.72107600	3.21130100
H	-4.62470100	-3.41918300	3.96052200
C	-3.59921200	-1.55547800	3.59502200
H	-3.44477600	-1.33942300	4.64967000
C	-3.12888700	-0.67049900	2.63174300
H	-2.60347600	0.22653500	2.95216500
B	-2.76220100	0.20721300	0.19650600

Compound (*M*)-**NPhBPy-HC** in S_0 state**.**

Total energy (PBE0-D3(BJ)/6-31G(d)) –2480.912817 a. u.

	X	Y	Z
N	-0.10371200	-0.19557400	-0.37579900
N	7.71715000	-0.56294700	0.06090600
C	-2.18073500	-1.43600200	-0.73896100
C	-4.36791100	-0.34659900	-1.08517800
C	-5.02327400	-1.61475500	-0.86483000
C	0.00883600	2.35740800	-0.83784300
C	0.79455000	3.24887600	-0.09413000
C	-4.22108800	-2.77576300	-0.90295100
C	-2.33787800	1.03295900	-0.86042900
C	-2.96526300	-0.23603600	-0.88147300
C	-0.71814700	-1.37266100	-0.64548600
C	-2.81160800	-2.65512300	-0.82037300
H	-2.25134900	-3.58370400	-0.78365300
C	-5.06937800	0.79858600	-1.51461200
H	-6.12121900	0.71486500	-1.76233500
C	0.11275500	2.43587800	-2.23554600
C	-4.82932000	-4.05356200	-1.05616600
H	-4.19309000	-4.93337900	-1.11277500
C	-6.87709000	0.28761000	0.78343400
C	1.64832100	4.16491200	-0.70813800
C	-7.01577200	-3.01813000	-1.02763000

C	6.33037700	-0.72378200	-0.06062000
C	-6.44131200	-1.77013300	-0.66559800
C	-5.64136400	0.25344900	1.46732100
H	-4.99690000	-0.61008900	1.36180300
C	-8.69545000	-0.84954500	-0.40432200
C	3.53474200	-1.04810300	-0.30029400
C	-3.08186800	2.13334200	-1.25144900
H	-2.60718700	3.11149700	-1.27282800
C	-7.75537500	1.37110000	1.06180500
C	2.08071000	-1.21371300	-0.42210600
C	-7.31403800	-0.75924400	-0.11846700
C	-9.22414600	-2.03905600	-0.97537900
H	-10.29307400	-2.09296800	-1.16630200
C	1.46433500	-2.43084500	-0.74530100
H	2.06736800	-3.31201000	-0.94503200
C	0.09249900	-2.50228700	-0.84956000
H	-0.36480300	-3.44098900	-1.13195700
C	-4.42666200	2.00951600	-1.63056900
H	-4.97447800	2.87795100	-1.98677400
C	5.52484000	0.32276200	-0.53217300
H	5.98262700	1.26700500	-0.80814700
C	1.22981300	-0.13440700	-0.24418000
H	1.61295900	0.84425400	0.01458500
C	-1.16052700	1.37640500	1.42656600
C	1.73771400	4.21255100	-2.09611100
C	4.15576000	0.15773700	-0.65619000
H	3.56219600	0.98000900	-1.04794600
C	8.42291600	-1.20560300	1.10368100
C	-5.23655600	1.28832500	2.27874300
H	-4.27333000	1.23598200	2.77709900
C	-6.17820700	-4.15286800	-1.21822600
H	-6.64440100	-5.10858800	-1.44372200
C	0.96181900	3.34339000	-2.86127500
C	-8.42308200	-3.12266800	-1.18582700
H	-8.84149000	-4.07098700	-1.51338900

C	-9.09431000	1.33635200	0.56970600
H	-9.75063400	2.17589900	0.78563100
C	-9.56226300	0.23752500	-0.07924700
H	-10.60675000	0.16762500	-0.37294100
C	8.42726000	0.25064900	-0.85143400
C	-6.06490600	2.40983400	2.45838600
H	-5.73096800	3.23505400	3.08131400
C	-7.31195400	2.43560600	1.87738900
H	-7.98873900	3.26815700	2.05583800
C	-0.96317500	0.36539800	2.37399600
C	5.71749000	-1.93629900	0.28650300
H	6.32608400	-2.75603300	0.65412400
C	4.34551300	-2.08703000	0.17330200
H	3.89448200	-3.02900100	0.47457600
C	7.90584100	-1.22493700	2.40326500
H	6.95597300	-0.73918500	2.60554700
C	9.65324700	-1.81816900	0.84522700
H	10.05264900	-1.80223700	-0.16428800
C	-1.69134000	2.58726300	1.89906400
B	-0.90364100	1.19735500	-0.16747600
C	8.60525900	-1.86077700	3.42181500
H	8.19247200	-1.86847700	4.42687000
C	9.42228300	1.11871600	-0.39100200
H	9.63406300	1.16760600	0.67274700
C	8.15118400	0.18779700	-2.22123500
H	7.38495200	-0.49321800	-2.57925200
C	9.83377600	-2.46519300	3.16590000
H	10.38138700	-2.95389200	3.96630000
C	10.35436200	-2.43467300	1.87441900
H	11.30959100	-2.90618400	1.66039500
C	-1.27433200	0.54575400	3.72174500
C	10.13094800	1.90570700	-1.29057700
H	10.90144100	2.57600700	-0.91965700
C	-1.99357500	2.78629600	3.24167000
C	-1.78799900	1.76043500	4.16373500

C	9.84754400	1.85273100	-2.65314400
H	10.39810200	2.47518600	-3.35224000
C	8.85178500	0.99314500	-3.11083200
H	8.62621500	0.93585100	-4.17214800
H	-0.49161300	1.76564500	-2.84458200
H	1.01873900	3.37627300	-3.94691000
H	-0.56051000	-0.59700200	2.06295100
H	-1.11137700	-0.26545300	4.42766000
H	-2.02702000	1.90783300	5.21385500
H	-2.39658600	3.74169800	3.57045900
H	-1.87591700	3.39333900	1.19194300
H	2.40193900	4.92464600	-2.57956100
H	2.24407400	4.84236300	-0.10062400
H	0.73880500	3.22122700	0.99215500

Compound (*M*)-**NFBPy-HC** in S_0 state**.**

Total energy (PBE0-D3(BJ)/6-31G(d)) –3472.329671 a. u.

	X	Y	Z
F	0.18213300	2.35197400	-1.87891500
F	-0.69321700	2.73973800	2.76773900
F	0.12721600	5.25892400	2.69271300
F	1.44727600	1.15425700	2.45754500
F	0.99387200	6.36905000	0.35935200
F	1.00628600	4.86506000	-1.91515100
F	-2.27727900	-1.54028800	1.31552300
N	-0.13291800	0.02600800	-0.69006500
F	1.80372300	-0.30045300	4.64456000
N	7.64910300	-0.95547700	-0.76657400
C	-2.24253400	-0.40634100	-1.85362800
C	-4.45794100	0.29607600	-1.01771200
C	-5.08875900	-0.48062500	-2.06277400
C	-0.24385300	2.37985200	0.46389800
C	-0.25397200	3.20494900	1.58676400
C	-4.26827900	-0.87618900	-3.14266700

C	-2.42340100	0.94284700	0.21561800
C	-3.04047800	0.27534600	-0.86682000
C	-0.79606300	-0.57437500	-1.70264200
C	-2.85997700	-0.85668400	-2.99564500
H	-2.28441700	-1.22990300	-3.83621200
F	0.13102800	-2.37180300	5.22280000
F	-1.91870300	-2.95792100	3.51566700
C	-5.20797900	1.12219200	-0.15868800
H	-6.27513000	1.22081300	-0.31599800
C	0.17685300	3.00980200	-0.70625500
C	-4.84918400	-1.28744000	-4.37328800
H	-4.19535300	-1.56199500	-5.19719100
C	-6.97606700	-1.22357300	0.35986000
C	0.15490300	4.53145000	1.57774500
C	-7.05105500	-0.99745000	-3.41807700
C	6.26073200	-0.91702700	-0.93464600
C	-6.49775800	-0.78398900	-2.12402300
C	-5.71566200	-1.78285300	0.67021500
H	-5.01906100	-2.00365100	-0.12876300
C	-8.77573400	-0.71195200	-1.22254900
C	3.45676400	-0.84029400	-1.27496400
C	-3.21959800	1.68772300	1.07028600
H	-2.76396600	2.20484200	1.90919000
C	-7.90125100	-1.06232800	1.43051000
C	1.99948500	-0.79842000	-1.44529400
C	-7.38989500	-0.87896400	-0.98838000
C	-9.28452800	-0.71832400	-2.54891600
H	-10.35617500	-0.60833400	-2.69412400
C	1.32138800	-1.48025400	-2.46835400
H	1.87712300	-2.08031200	-3.18299200
C	-0.04565900	-1.37634800	-2.58111600
H	-0.55319700	-1.92667600	-3.36153500
C	-4.59806100	1.81073700	0.86379800
H	-5.19068400	2.44726200	1.51502400
C	5.52815700	0.23128900	-0.59864600

H	6.04589600	1.09941700	-0.20457500
C	1.20130700	-0.08252000	-0.57104900
H	1.62720200	0.42777800	0.28447700
C	-0.51667100	-0.02769800	1.82639600
C	0.59553000	5.10100200	0.39126200
C	4.15563000	0.26618300	-0.77346400
H	3.61863100	1.17869800	-0.52819200
C	8.29840100	-2.16629600	-0.43031700
C	-5.35194500	-2.07121500	1.96714600
H	-4.37057500	-2.48645700	2.17038300
C	-6.20045900	-1.25192400	-4.52908900
H	-6.65811400	-1.46107800	-5.49245300
C	0.60316500	4.33206500	-0.76228500
C	-8.45721400	-0.95351600	-3.60484600
H	-8.85223800	-1.07032100	-4.61065200
C	-9.24889500	-0.68719900	1.15480600
H	-9.93499600	-0.55747600	1.98803900
C	-9.68129100	-0.57895300	-0.12749300
H	-10.72745400	-0.38268800	-0.34843600
C	8.42495200	0.21681500	-0.92611100
C	-6.23918600	-1.81844900	3.02649300
H	-5.94011400	-2.03017600	4.04915600
C	-7.49854400	-1.33783700	2.75505100
H	-8.21735400	-1.18450000	3.55657000
C	0.54391000	0.18871200	2.70307200
C	5.56894800	-2.02573500	-1.44526500
H	6.11920200	-2.92282500	-1.70923600
C	4.19436100	-1.98425600	-1.60487400
H	3.68377600	-2.86782500	-1.97898700
C	7.76466400	-3.00835100	0.55054700
H	6.84581200	-2.72375500	1.05448200
C	9.49047600	-2.52262700	-1.06813200
H	9.90277600	-1.86620600	-1.82841900
C	-1.29779800	-1.14050200	2.13783600
B	-0.84691500	0.85849600	0.48005900

C	8.40946900	-4.19601300	0.87423800
H	7.98509200	-4.84151500	1.63824800
C	9.44659800	0.51009600	-0.01797300
H	9.62781000	-0.16382500	0.81380300
C	8.18772700	1.08308000	-1.99806900
H	7.40088900	0.84854500	-2.70876900
C	9.60010100	-4.54854200	0.24322000
H	10.10569600	-5.47329600	0.50497300
C	10.13807000	-3.70295600	-0.72394700
H	11.06436600	-3.96847000	-1.22591100
C	0.77493400	-0.57096800	3.84327300
C	10.21996900	1.65237400	-0.18579100
H	11.01077700	1.86973100	0.52679400
C	-1.11312300	-1.92269100	3.27050000
C	-0.07112300	-1.63098300	4.13826000
C	9.97546100	2.52252600	-1.24539300
H	10.57662600	3.41845300	-1.36851000
C	8.95352400	2.23309800	-2.14636300
H	8.75817100	2.89939900	-2.98202000

Compound (*M*)-**BiNFBPy-HC** in S_0 state**.**

Total energy (PBE0-D3(BJ)/6-31G(d)) –5945.319165 a. u.

	X	Y	Z
F	2.22883200	6.17452300	1.87110900
F	2.08715500	3.52981000	-2.06501600
F	4.47412300	4.45625000	-2.75052000
F	0.30565800	5.51280500	-2.33978600
F	5.77626800	6.24964300	-1.16466900
F	4.60453200	7.08759400	1.15054500
F	-1.72669000	2.41519300	0.61110500
N	-0.17970600	5.27523100	1.31814800
F	-1.46206300	4.86386400	-4.20599000
N	-2.12015100	12.33901100	-1.48428800
C	-0.17985000	3.79492900	3.26854300

C	0.67067200	1.47348000	3.25096700
C	0.12694600	1.27708100	4.57788000
C	1.99084000	4.84519400	-0.09057800
C	2.65095200	4.43222700	-1.24633900
C	-0.22163000	2.43861400	5.30239400
C	0.87896700	2.87230600	1.23049600
C	0.45170600	2.70654700	2.56737400
C	-0.54604600	5.04497600	2.59773300
C	-0.39140800	3.66785900	4.61972900
H	-0.71479700	4.51079700	5.22118000
F	-3.36719100	2.97886000	-3.71899400
F	-3.45970400	1.76492800	-1.27335000
C	1.45253900	0.48983500	2.61434300
H	1.70349100	-0.41864500	3.14799700
C	2.71749200	5.73645400	0.69717000
C	-0.40360000	2.38071600	6.71100800
H	-0.64194400	3.29663800	7.24589300
C	3.90664900	4.88666200	-1.62573600
C	0.00000000	0.00000000	6.66352100
C	-1.88085100	11.14617200	-0.79416600
C	0.00000000	0.00000000	5.23916200
C	-1.40105200	8.73458600	0.59898200
C	1.58686100	1.84246000	0.63292200
H	1.91823100	1.94918900	-0.39551600
C	-1.15209200	7.47778700	1.31486800
C	-1.59403200	7.23375200	2.62475300
H	-2.15348900	7.99483000	3.16076700
C	-1.30530700	6.03810900	3.24125500
H	-1.67445500	5.85944100	4.24187800
C	1.90782100	0.67217700	1.32863400
H	2.49874900	-0.09978500	0.84689000
C	-0.71148400	10.40535300	-1.02284200
H	0.01627500	10.76353500	-1.74325700
C	-0.46998400	6.43714100	0.70926900
H	-0.14096500	6.50802800	-0.32047900

C	-0.52712300	3.90422600	-0.79963100
C	4.57370300	5.79901200	-0.82017000
C	-0.47810400	9.22844400	-0.33302400
H	0.44849400	8.69006000	-0.51386300
C	-3.44084500	12.72844500	-1.80913100
C	-0.20486700	1.21099000	7.37807500
H	-0.24399700	1.17224200	8.46343200
C	3.97319500	6.22501900	0.35449600
C	-1.04578500	13.17182100	-1.87675000
C	-0.56386200	4.53005500	-2.04346300
C	-2.80505900	10.66294200	0.14455100
H	-3.71552000	11.22188300	0.33377200
C	-2.56730700	9.47808600	0.81980700
H	-3.31476400	9.11671000	1.52125000
C	-4.34896500	11.79722900	-2.32295300
H	-4.03123200	10.76963800	-2.47243900
C	-3.84261800	14.05582600	-1.63232200
H	-3.13444500	14.77640400	-1.23457300
C	-1.56569500	2.99842700	-0.58434800
B	0.56679300	4.19918000	0.39231100
C	-5.64413300	12.18955200	-2.63889800
H	-6.34035500	11.45697100	-3.03771800
C	-1.03092100	13.74028200	-3.15387900
H	-1.84383900	13.52516900	-3.84070700
C	0.00000000	13.44552700	-0.98953900
H	-0.01837400	13.01188200	0.00587600
C	-6.04320800	13.51303200	-2.46798500
H	-7.05359800	13.81770700	-2.72411900
C	-5.13407300	14.44280200	-1.96913300
H	-5.43431400	15.47743900	-1.82817300
C	-1.49211700	4.23288500	-3.03350000
C	0.01506900	14.57295400	-3.53272200
H	0.01574300	15.00834800	-4.52812300
C	-2.50938900	2.66032000	-1.54563000
C	-2.46833400	3.27722800	-2.78735700

C	1.06377700	14.83507700	-2.65453400
H	1.88364300	15.47968100	-2.95711300
C	1.05150800	14.26376500	-1.38435700
H	1.85940400	14.46716500	-0.68695000
F	-2.22883200	-6.17452300	1.87110900
F	-2.08715500	-3.52981000	-2.06501600
F	-4.47412300	-4.45625000	-2.75052000
F	-0.30565800	-5.51280500	-2.33978600
F	-5.77626800	-6.24964300	-1.16466900
F	-4.60453200	-7.08759400	1.15054500
F	1.72669000	-2.41519300	0.61110500
N	0.17970600	-5.27523100	1.31814800
F	1.46206300	-4.86386400	-4.20599000
N	2.12015100	-12.33901100	-1.48428800
C	0.17985000	-3.79492900	3.26854300
C	-0.67067200	-1.47348000	3.25096700
C	-0.12694600	-1.27708100	4.57788000
C	-1.99084000	-4.84519400	-0.09057800
C	-2.65095200	-4.43222700	-1.24633900
C	0.22163000	-2.43861400	5.30239400
C	-0.87896700	-2.87230600	1.23049600
C	-0.45170600	-2.70654700	2.56737400
C	0.54604600	-5.04497600	2.59773300
C	0.39140800	-3.66785900	4.61972900
H	0.71479700	-4.51079700	5.22118000
F	3.36719100	-2.97886000	-3.71899400
F	3.45970400	-1.76492800	-1.27335000
C	-1.45253900	-0.48983500	2.61434300
H	-1.70349100	0.41864500	3.14799700
C	-2.71749200	-5.73645400	0.69717000
C	0.40360000	-2.38071600	6.71100800
H	0.64194400	-3.29663800	7.24589300
C	-3.90664900	-4.88666200	-1.62573600
C	1.88085100	-11.14617200	-0.79416600
C	1.40105200	-8.73458600	0.59898200

C	-1.58686100	-1.84246000	0.63292200
H	-1.91823100	-1.94918900	-0.39551600
C	1.15209200	-7.47778700	1.31486800
C	1.59403200	-7.23375200	2.62475300
H	2.15348900	-7.99483000	3.16076700
C	1.30530700	-6.03810900	3.24125500
H	1.67445500	-5.85944100	4.24187800
C	-1.90782100	-0.67217700	1.32863400
H	-2.49874900	0.09978500	0.84689000
C	0.71148400	-10.40535300	-1.02284200
H	-0.01627500	-10.76353500	-1.74325700
C	0.46998400	-6.43714100	0.70926900
H	0.14096500	-6.50802800	-0.32047900
C	0.52712300	-3.90422600	-0.79963100
C	-4.57370300	-5.79901200	-0.82017000
C	0.47810400	-9.22844400	-0.33302400
H	-0.44849400	-8.69006000	-0.51386300
C	3.44084500	-12.72844500	-1.80913100
C	0.20486700	-1.21099000	7.37807500
H	0.24399700	-1.17224200	8.46343200
C	-3.97319500	-6.22501900	0.35449600
C	1.04578500	-13.17182100	-1.87675000
C	0.56386200	-4.53005500	-2.04346300
C	2.80505900	-10.66294200	0.14455100
H	3.71552000	-11.22188300	0.33377200
C	2.56730700	-9.47808600	0.81980700
H	3.31476400	-9.11671000	1.52125000
C	4.34896500	-11.79722900	-2.32295300
H	4.03123200	-10.76963800	-2.47243900
C	3.84261800	-14.05582600	-1.63232200
H	3.13444500	-14.77640400	-1.23457300
C	1.56569500	-2.99842700	-0.58434800
B	-0.56679300	-4.19918000	0.39231100
C	5.64413300	-12.18955200	-2.63889800
H	6.34035500	-11.45697100	-3.03771800

C	1.03092100	-13.74028200	-3.15387900
H	1.84383900	-13.52516900	-3.84070700
C	0.00000000	-13.44552700	-0.98953900
H	0.01837400	-13.01188200	0.00587600
C	6.04320800	-13.51303200	-2.46798500
H	7.05359800	-13.81770700	-2.72411900
C	5.13407300	-14.44280200	-1.96913300
H	5.43431400	-15.47743900	-1.82817300
C	1.49211700	-4.23288500	-3.03350000
C	-0.01506900	-14.57295400	-3.53272200
H	-0.01574300	-15.00834800	-4.52812300
C	2.50938900	-2.66032000	-1.54563000
C	2.46833400	-3.27722800	-2.78735700
C	-1.06377700	-14.83507700	-2.65453400
H	-1.88364300	-15.47968100	-2.95711300
C	-1.05150800	-14.26376500	-1.38435700
H	-1.85940400	-14.46716500	-0.68695000

Compound (*M*)-**NFBPy-HC** in S_1 state**.**

Total energy (PBE0-D3(BJ)/6-31G(d)) –3472.239421 a. u.

	X	Y	Z
F	-0.04432433	2.50061985	-1.78733680
F	-0.73684353	2.60736141	2.90528466
F	-0.03365571	5.16278969	2.93081116
F	1.46672033	1.13134606	2.47510270
F	0.68091457	6.42839468	0.62628821
F	0.66448080	5.04917209	-1.72245012
F	-2.22834713	-1.59440750	1.32175846
N	-0.11982204	0.08945962	-0.67988505
F	1.94317469	-0.43170821	4.56693551
N	7.66209482	-0.90910571	-0.81868538
C	-2.21080326	-0.26155474	-1.91527587
C	-4.44063687	0.31058078	-0.99090618
C	-5.08180536	-0.37342133	-2.08350339

C	-0.35651626	2.38426879	0.56927137
C	-0.36540575	3.15107150	1.73386716
C	-4.25643865	-0.63316439	-3.22531353
C	-2.41729763	0.86883681	0.27656143
C	-3.02617747	0.30852263	-0.86635348
C	-0.79444660	-0.43010176	-1.77399656
C	-2.86176980	-0.58631783	-3.11193945
H	-2.28729293	-0.80530619	-4.00589667
F	0.34907550	-2.57772604	5.08869940
F	-1.75053578	-3.12728262	3.42875494
C	-5.19400819	1.04732697	-0.05016683
H	-6.25931726	1.16669810	-0.21117303
C	-0.02297213	3.09280362	-0.58619181
C	-4.87989665	-0.91355685	-4.47498633
H	-4.25212648	-1.06721763	-5.34873636
C	-6.86632304	-1.38908306	0.31069183
C	-0.01771096	4.49361091	1.77940361
C	-7.06860337	-0.81279900	-3.42479666
C	6.26912239	-0.84171614	-0.99708607
C	-6.47390472	-0.70593143	-2.13262319
C	-5.59673369	-1.97381484	0.52293395
H	-4.92864936	-2.11460569	-0.31830991
C	-8.72797628	-0.74937758	-1.15992176
C	3.46490957	-0.70820395	-1.35211491
C	-3.22587567	1.51405282	1.23319514
H	-2.75732369	1.94352923	2.11267503
C	-7.75375652	-1.32867349	1.42325055
C	2.01583412	-0.65087907	-1.52563135
C	-7.32798325	-0.92101143	-0.98440139
C	-9.27740858	-0.65313662	-2.46076492
H	-10.35380162	-0.54783908	-2.56648276
C	1.33314833	-1.27001469	-2.61610020
H	1.88625175	-1.81295534	-3.37504884
C	-0.02545116	-1.14660964	-2.71835664
H	-0.53766054	-1.62802585	-3.54246871

C	-4.59558985	1.62990297	1.05764573
H	-5.20122310	2.17554419	1.77495079
C	5.52978483	0.22091879	-0.45702265
H	6.04162898	0.99767113	0.10231353
C	1.21751867	-0.01503076	-0.59799624
H	1.65045877	0.42770218	0.29115810
C	-0.47458007	-0.08477876	1.84235164
C	0.34468673	5.14267229	0.60696652
C	4.16188205	0.28784005	-0.64304669
H	3.62206285	1.13988158	-0.24030611
C	8.28075012	-2.15161207	-0.57689911
C	-5.19119189	-2.38318608	1.77461207
H	-4.20558890	-2.81582920	1.90649152
C	-6.23694666	-0.92143884	-4.57808359
H	-6.71712866	-1.05155472	-5.54494009
C	0.33872048	4.43542151	-0.58593114
C	-8.47266921	-0.78222539	-3.56174244
H	-8.89960788	-0.81394425	-4.56104882
C	-9.11088280	-0.93376822	1.22779160
H	-9.76743444	-0.88244261	2.09285827
C	-9.59093197	-0.71488772	-0.02316587
H	-10.64511883	-0.50589753	-0.18669326
C	8.43750649	0.26581102	-0.87506993
C	-6.03923991	-2.22772613	2.88346327
H	-5.70482100	-2.53276062	3.87094708
C	-7.30625550	-1.72302444	2.70144101
H	-7.99591649	-1.64358757	3.53857486
C	0.60555691	0.12232677	2.69571605
C	5.59300193	-1.83273626	-1.72121599
H	6.15453710	-2.65843575	-2.14712791
C	4.22107795	-1.76552212	-1.88805718
H	3.72163603	-2.56224081	-2.43122302
C	7.66390915	-3.09749237	0.25183551
H	6.71192606	-2.85856209	0.71552991
C	9.51614647	-2.45288929	-1.16416699

H	9.98861640	-1.72329584	-1.81444372
C	-1.22126124	-1.22626978	2.12640397
B	-0.83572989	0.81224680	0.51321136
C	8.27334576	-4.32396362	0.48007251
H	7.78657000	-5.04734630	1.12812251
C	9.50721497	0.45083036	0.01006319
H	9.72820441	-0.31573540	0.74616859
C	8.14219728	1.26151449	-1.81496965
H	7.31895454	1.11321187	-2.50681221
C	9.50562061	-4.62107849	-0.09848725
H	9.98114860	-5.57944166	0.08731400
C	10.12253481	-3.67727607	-0.91720768
H	11.07932363	-3.90036854	-1.38099418
C	0.89629130	-0.69037706	3.78476330
C	10.26876405	1.60996969	-0.05338088
H	11.09313209	1.74356717	0.64146810
C	-0.97727834	-2.06226887	3.20760400
C	0.08933520	-1.78787133	4.05142092
C	9.97041053	2.60380164	-0.98343134
H	10.56457742	3.51172718	-1.02455450
C	8.90195007	2.42278831	-1.85918106
H	8.66384005	3.18662642	-2.59404981

Compound (*M*)-**BiNFBPy-HC** in S_1 state**.**

Total energy (PBE0-D3(BJ)/6-31G(d)) –5945.229241 a. u.

	X	Y	Z
F	-0.40042356	6.47911384	1.98681770
F	0.70961143	4.02035580	-1.91651204
F	2.53984867	5.84019872	-2.51865419
F	-1.70397689	5.09976248	-2.31668344
F	2.93231259	8.00149106	-0.90592813
F	1.42641066	8.28191605	1.34843021
F	-2.43306485	1.46519537	0.62511356
N	-2.22270871	4.68483568	1.33502079

F	-2.98415507	3.78291711	-4.23138205
N	-6.90050885	10.21444030	-1.67357229
C	-1.66223518	3.38278834	3.33216980
C	0.06533698	1.61020777	3.37456360
C	-0.38145728	1.21531062	4.69045093
C	-0.00000000	5.17822582	0.03261833
C	0.82150678	5.07183642	-1.08848840
C	-1.17814984	2.16103896	5.40460324
C	-0.27465068	2.93654803	1.33200856
C	-0.62362951	2.63709562	2.66672704
C	-2.48779725	4.33993454	2.63213919
C	-1.81423374	3.19872898	4.70339713
H	-2.44280546	3.86418621	5.28532516
F	-3.98723430	1.29301341	-3.77260963
F	-3.68300965	0.15562847	-1.30610174
C	1.20418268	1.03208305	2.77945312
H	1.80069575	0.32900252	3.34956024
C	0.26916789	6.28340059	0.83954123
C	-1.30891252	2.03965514	6.81628267
H	-1.87884166	2.79254590	7.35388188
C	1.79872568	5.99869117	-1.42390264
C	-0.00000000	-0.00000000	6.78446297
C	-6.19216758	9.24912533	-0.94563472
C	-0.00000000	-0.00000000	5.35198947
C	-4.76364377	7.29786836	0.52223529
C	0.81314353	2.27352494	0.76381690
H	1.09060731	2.49306061	-0.26239608
C	-4.02753162	6.28174247	1.27381314
C	-4.36428171	5.88852260	2.59119540
H	-5.20616808	6.34689530	3.10056753
C	-3.61131906	4.94335132	3.23818925
H	-3.89234861	4.64093270	4.23845724
C	1.57329456	1.35804882	1.48872273
H	2.44095968	0.89272460	1.03501248
C	-4.83189846	9.01494047	-1.19895976

H	-4.32469445	9.58943006	-1.96719309
C	-2.95692409	5.61463565	0.70615858
H	-2.66399802	5.80505003	-0.31953205
C	-1.88186647	3.29853533	-0.77584967
C	2.00273750	7.10003148	-0.60420752
C	-4.13608271	8.06620383	-0.47295466
H	-3.07727755	7.92919650	-0.67374745
C	-8.25676373	10.00282523	-2.00462966
C	-0.66597184	1.03594110	7.48405816
H	-0.69084221	0.99210843	8.57019790
C	1.23202219	7.24072023	0.53964219
C	-6.26288815	11.40409971	-2.08872441
C	-2.11478671	3.85117429	-2.03239193
C	-6.82706222	8.49743132	0.05423501
H	-7.87834998	8.66762218	0.26300781
C	-6.12481797	7.54113035	0.76575306
H	-6.65157932	6.95756241	1.51548173
C	-8.69149707	8.74466716	-2.43683978
H	-7.97466071	7.93371880	-2.52248591
C	-9.17571066	11.05384936	-1.91005368
H	-8.83668553	12.02777876	-1.57069394
C	-2.47496812	2.05268909	-0.57880900
B	-1.07543642	4.01783039	0.46312963
C	-10.02806291	8.54340333	-2.75708818
H	-10.35292752	7.56293287	-3.09387798
C	-6.49746830	11.91790341	-3.36893018
H	-7.16458385	11.38734458	-4.04126062
C	-5.39720106	12.08168747	-1.22265072
H	-5.22452864	11.68756605	-0.22581875
C	-10.94218306	9.59094430	-2.66860804
H	-11.98478041	9.43108991	-2.92673527
C	-10.50672390	10.84576919	-2.24837659
H	-11.21118973	11.66912215	-2.16980212
C	-2.80469806	3.19950769	-3.04744428
C	-5.87697696	13.09409367	-3.76993510

H	-6.06470820	13.48181104	-4.76728314
C	-3.16300478	1.35700192	-1.56385629
C	-3.32308387	1.93268163	-2.81595270
C	-5.00687477	13.76331365	-2.91214177
H	-4.51807964	14.67851491	-3.23247941
C	-4.76901006	13.24816696	-1.63987072
H	-4.09906990	13.76516683	-0.95858836
F	0.40042356	-6.47911384	1.98681770
F	-0.70961143	-4.02035580	-1.91651204
F	-2.53984867	-5.84019872	-2.51865419
F	1.70397689	-5.09976248	-2.31668344
F	-2.93231259	-8.00149106	-0.90592813
F	-1.42641066	-8.28191605	1.34843021
F	2.43306485	-1.46519537	0.62511356
N	2.22270871	-4.68483568	1.33502079
F	2.98415507	-3.78291711	-4.23138205
N	6.90050885	-10.21444030	-1.67357229
C	1.66223518	-3.38278834	3.33216980
C	-0.06533698	-1.61020777	3.37456360
C	0.38145728	-1.21531062	4.69045093
C	0.00000000	-5.17822582	0.03261833
C	-0.82150678	-5.07183642	-1.08848840
C	1.17814984	-2.16103896	5.40460324
C	0.27465068	-2.93654803	1.33200856
C	0.62362951	-2.63709562	2.66672704
C	2.48779725	-4.33993454	2.63213919
C	1.81423374	-3.19872898	4.70339713
H	2.44280546	-3.86418621	5.28532516
F	3.98723430	-1.29301341	-3.77260963
F	3.68300965	-0.15562847	-1.30610174
C	-1.20418268	-1.03208305	2.77945312
H	-1.80069575	-0.32900252	3.34956024
C	-0.26916789	-6.28340059	0.83954123
C	1.30891252	-2.03965514	6.81628267
H	1.87884166	-2.79254590	7.35388188

C	-1.79872568	-5.99869117	-1.42390264
C	6.19216758	-9.24912533	-0.94563472
C	4.76364377	-7.29786836	0.52223529
C	-0.81314353	-2.27352494	0.76381690
H	-1.09060731	-2.49306061	-0.26239608
C	4.02753162	-6.28174247	1.27381314
C	4.36428171	-5.88852260	2.59119540
H	5.20616808	-6.34689530	3.10056753
C	3.61131906	-4.94335132	3.23818925
H	3.89234861	-4.64093270	4.23845724
C	-1.57329456	-1.35804882	1.48872273
H	-2.44095968	-0.89272460	1.03501248
C	4.83189846	-9.01494047	-1.19895976
H	4.32469445	-9.58943006	-1.96719309
C	2.95692409	-5.61463565	0.70615858
H	2.66399802	-5.80505003	-0.31953205
C	1.88186647	-3.29853533	-0.77584967
C	-2.00273750	-7.10003148	-0.60420752
C	4.13608271	-8.06620383	-0.47295466
H	3.07727755	-7.92919650	-0.67374745
C	8.25676373	-10.00282523	-2.00462966
C	0.66597184	-1.03594110	7.48405816
H	0.69084221	-0.99210843	8.57019790
C	-1.23202219	-7.24072023	0.53964219
C	6.26288815	-11.40409971	-2.08872441
C	2.11478671	-3.85117429	-2.03239193
C	6.82706222	-8.49743132	0.05423501
H	7.87834998	-8.66762218	0.26300781
C	6.12481797	-7.54113035	0.76575306
H	6.65157932	-6.95756241	1.51548173
C	8.69149707	-8.74466716	-2.43683978
H	7.97466071	-7.93371880	-2.52248591
C	9.17571066	-11.05384936	-1.91005368
H	8.83668553	-12.02777876	-1.57069394
C	2.47496812	-2.05268909	-0.57880900

B	1.07543642	-4.01783039	0.46312963
C	10.02806291	-8.54340333	-2.75708818
H	10.35292752	-7.56293287	-3.09387798
C	6.49746830	-11.91790341	-3.36893018
H	7.16458385	-11.38734458	-4.04126062
C	5.39720106	-12.08168747	-1.22265072
H	5.22452864	-11.68756605	-0.22581875
C	10.94218306	-9.59094430	-2.66860804
H	11.98478041	-9.43108991	-2.92673527
C	10.50672390	-10.84576919	-2.24837659
H	11.21118973	-11.66912215	-2.16980212
C	2.80469806	-3.19950769	-3.04744428
C	5.87697696	-13.09409367	-3.76993510
H	6.06470820	-13.48181104	-4.76728314
C	3.16300478	-1.35700192	-1.56385629
C	3.32308387	-1.93268163	-2.81595270
C	5.00687477	-13.76331365	-2.91214177
H	4.51807964	-14.67851491	-3.23247941
C	4.76901006	-13.24816696	-1.63987072
H	4.09906990	-13.76516683	-0.95858836