

# ADVANCED OPTICAL MATERIALS

## Supporting Information

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Interplay of Excited-States on Circularly Polarized Thermally Activated Delayed Fluorescent Chiral Exciplexes

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# Electronic Supplementary Information

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## A. General methods

$^1\text{H}$  and  $^{13}\text{C}$  NMR spectra were recorded at room temperature on an AVANCE III 400 BRUKER or an AVANCE I 500 BRUKER at Centre Régional de Mesures Physiques de l'Ouest (CRMPO), Université de Rennes. Chemical shifts  $\delta$  are given in ppm and coupling constants  $J$  in Hz. Chemical shifts for  $^1\text{H}$  NMR spectra are referenced relative to residual protium in the deuterated solvent ( $\delta = 7.26$  ppm,  $\text{CDCl}_3$ ),  $^{13}\text{C}$  shifts are referenced to  $\text{CDCl}_3$  peaks at  $\delta = 77.16$  ppm.

High-resolution mass (HR-MS) determinations were performed at CRMPO on a Bruker MaXis 4G by ASAP (+ or -) or ESI and MALDI with dichloromethane as solvent techniques. Experimental and calculated masses are given with consideration of the mass of the electron.

UV-Visible (UV-vis, in  $\text{M}^{-1} \text{cm}^{-1}$ ) absorption spectra were recorded on a UV-2401PC Shimadzu spectrophotometer.

Steady-state luminescence spectra were measured using an Edinburgh FS920 Steady State Fluorimeter combined with a FL920 Fluorescence Lifetime Spectrometer. The spectra were corrected for the wavelength dependence of the detector, and the quoted emission maxima refer to the values after correction. Life-times measurements were conducted with 375 nm diode laser excitation (EPL-series) plugged to a TCSPC pulsed source interface. Absolute fluorescence quantum yields  $\phi$  were recorded with a Hamamatsu C9920-03 integrating sphere.

For the vacuum luminescence measurement, a piece of the glass substrate was placed in a nmr tube with a J. Young valve, which can be freed from oxygen with a residual pressure of  $\sim 10^{-2}$  mbar. Then the tube can be placed in a dedicated holder for fluorescence measurements.

The thin films used in this study have been prepared on glass substrates by spin coating solutions of either the pure donor compound, or a mixture of the donor and acceptor molecules in the indicated weight ratio, all being at a concentration of  $\sim 10 \text{ mg}\cdot\text{mL}^{-1}$ . 0.1 mL of the solution is deposited on the glass fixed within the spin-coater holder, and the film is obtained using a sequence including 60 seconds of rotation, with an acceleration of  $500 \text{ rpm}\cdot\text{s}^{-1}$  and a maximum speed of 2000 rpm.

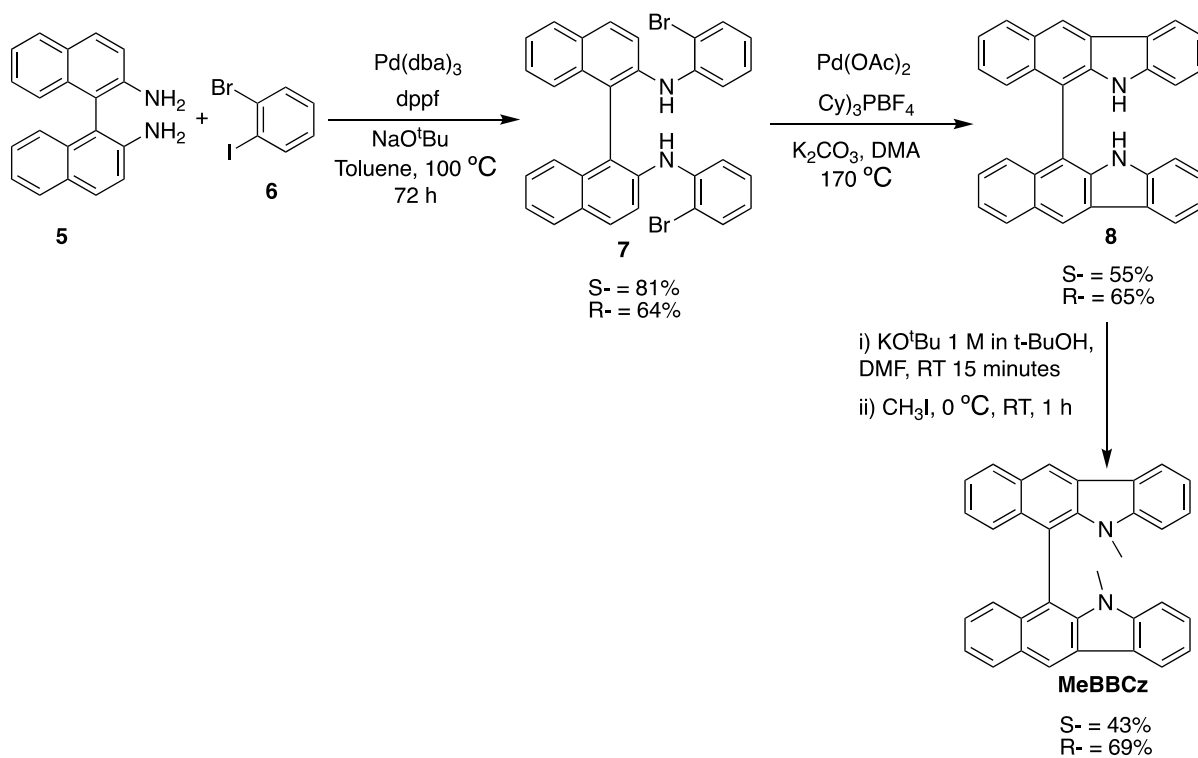
Electrochemical measurements were performed with a potentiostat PGSTAT 302N controlled by resident GPES (General Purpose Electrochemical System 4.9) software using a conventional single auxiliary electrode were platinum electrode potassium chloride calomel electrode (SCE). The supporting electrolyte was 0.2 N  $\text{Bu}_4\text{NPF}_6$  (tetrabutylammonium hexafluorophosphate) in dichloromethane and solutions were purged with argon before the measurements. All potentials are quoted relative to SCE, and the scan rate was either 100, 200 or 400 mV/s.

Electronic circular dichroism (ECD, in  $\text{M}^{-1} \text{cm}^{-1}$ ) was measured on a Jasco J-815 Circular Dichroism Spectrometer (IFR140 facility - Biosit - Université de Rennes 1).

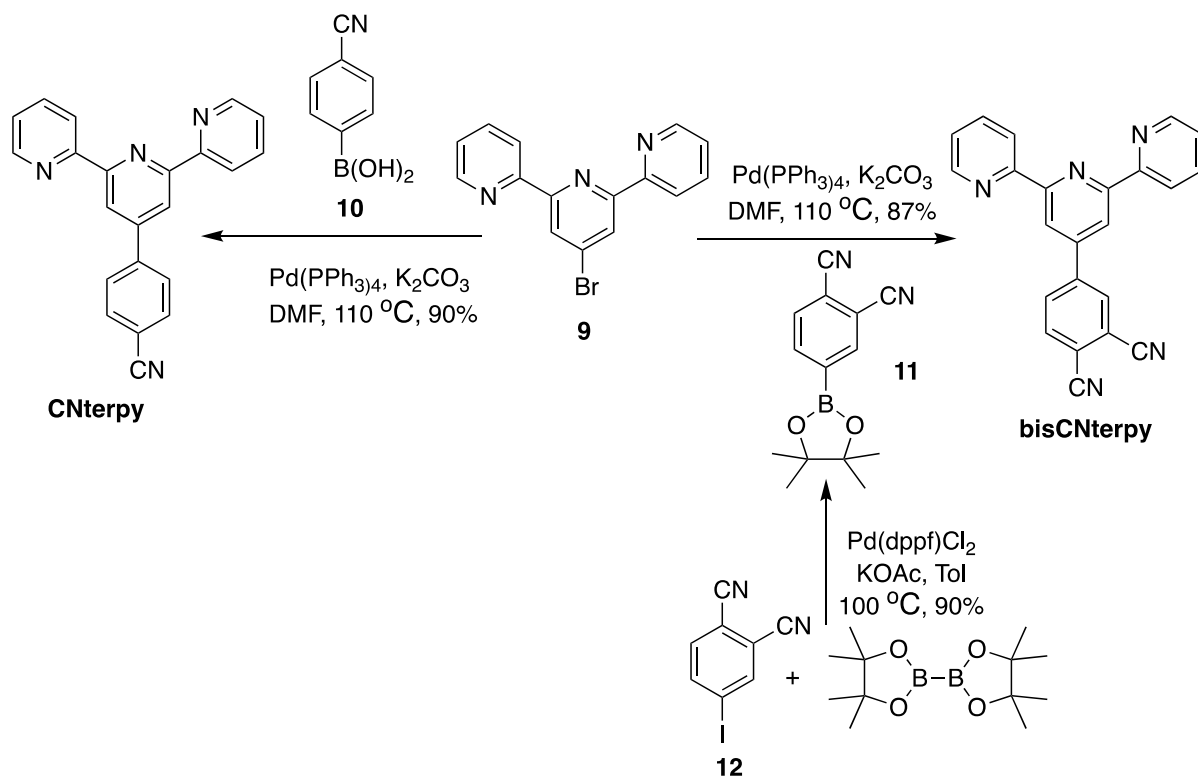
The circularly polarized luminescence (CPL) measurements were performed using a home-built CPL spectrofluoropolarimeter (constructed with the help of the JASCO Company). The samples were excited using a  $90^\circ$  geometry with a Xenon ozone-free lamp 150 W LS. The following parameters were used: emission slit width  $\approx 2$  mm, integration time = 4 sec, scan speed = 50 nm/min, accumulations = 10. The concentration of all the samples was ca.  $10^{-6}$  M.

Thin-layer chromatography (TLC) was performed on aluminum sheets precoated with Merck 5735 Kieselgel 60F254. Column chromatography was carried out with Merck 5735 Kieselgel 60F (0.040-0.063 mm mesh). Chemicals were purchased from Sigma-Aldrich, Alfa Aesar or TCI Europe and used as received.

## B. Synthetic procedures

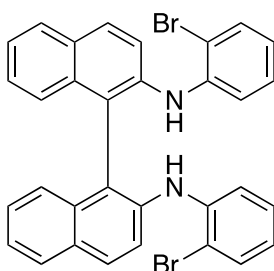


**Scheme S1.** Synthetic pathways of (*R*)- and (*S*)-MeBBCz.



**Scheme S2.** Synthetic route of CNterpy and BisCNterpy.

### **N<sup>2</sup>,N<sup>2'</sup>-bis(2-bromophenyl)-[1,1'-binaphthalene]-2,2'-diamine (7)**



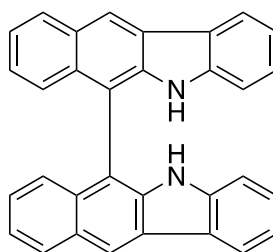
Tris(dibenzylideneacetone)dipalladium(0) (140 mg, 0.15 mmol), sodium *tert*-butoxide (2.40 g, 25 mmol), 1,1'-Bis(diphenylphosphino)ferrocene (dppf) (275 mg, 0.5 mmol) (*S*)-2,2'-diamino-1,1'-binaphthene **5** (*S*)-BINAM; 1.42 g, 5 mmol), were placed in a round bottom flask under a argon atmosphere and 1-bromo-2-iodobenzene **6** (3.185 mL, 25 mmol) and dissolved in dry toluene (15 mL) were added. The mixture was stirred at 120 °C for 72 h. Consumption of (*S*)-BINAM was monitored by Thin layer Chromatography (TLC). After the reaction mixture was cooling to room temperature, the mixture was diluted with DCM and filtered through celite with excess of DCM, and then concentrated under vacuum. The obtained crude product was purified by chromatography on silica gel with 3-6% of Ethyl acetate in n-heptane to give the titled compound **3** obtained as a pale yellowish white solid (2.39 mg, 81% yield). The (*R*) enantiomer was also prepared by using this procedure (64% yield).

<sup>1</sup>H NMR (400 MHz, CDCl<sub>3</sub>) δ 7.94 (d, *J* = 9.0 Hz, 2H), 7.88 (d, *J* = 8.0 Hz, 2H), 7.68 (d, *J* = 8.9 Hz, 2H), 7.40 – 7.31 (m, 4H), 7.31 – 7.19 (m, 6H), 7.14 – 7.01 (m, 2H), 6.67 (ddd, *J* = 7.9, 7.4, 1.5 Hz, 2H), 5.87 (s, 2H).

<sup>13</sup>C NMR (400 MHz, CDCl<sub>3</sub>) δ 140.4, 138.5, 133.8, 132.7, 129.9, 129.4, 128.2, 127.9, 127.1, 124.6, 124.1, 121.7, 119.1, 118.7, 117.1, 113.8.

HRMS (ESI): *m/z* calculated for C<sub>32</sub>H<sub>22</sub>Br<sub>2</sub>N<sub>2</sub> [M+H]<sup>+</sup>: 593.0228, found [M+H]<sup>+</sup>: 593.0233.

### **5H,5'H-6,6'-bibenzo[b]carbazole (8)**



Under argon atmosphere, (*S*)-*N*2,*N*2'-bis(2-bromophenyl)-[1,1'-binaphthalene]-2,2'-diamine **7** (1.50 g, 2.553 mmol), tricyclohexylphosphine tetrafluoroborate (187 mg, 0.5 mmol), Pd(OAc)<sub>2</sub> (57 mg, 0.25 mmol) and K<sub>2</sub>CO<sub>3</sub> (1.40 g, 10.2 mmol) were taken in round bottom flask and anhydrous *N,N*-Dimethylacetamide (DMA) (30 mL) was added at RT. The reaction mixture

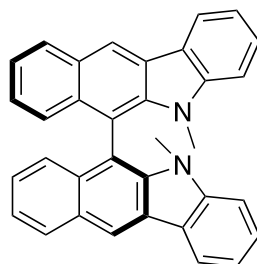
was stirred at 170 °C for 24 hours. Then, the reaction mixture was diluted with chloroform and filtered through celite using excess of chloroform. The filtered solution was concentrated in vacuum and purified by silica gel column chromatography using 15-20% DCM in n-heptane solvent mixture. The desired dibenzocarbazole (*S*)-**8** was obtained as pale yellowish white solid. (605 mg, 55% yield). The (*R*)-enantiomer was also prepared by using this procedure (65% yield).

<sup>1</sup>H NMR (400 MHz, CDCl<sub>3</sub>) δ 8.80 (s, 2H), 8.31 (d, *J* = 7.8 Hz, 2H), 8.24 (dd, *J* = 8.9, 0.9 Hz, 2H), 7.51 – 7.39 (m, 8H), 7.33 – 7.25 (m, 4H), 7.16 (d, *J* = 8.0 Hz, 2H).

<sup>13</sup>C NMR (400 MHz, CDCl<sub>3</sub>) δ 144.3, 140.0, 133.7, 128.5, 127.8, 127.3, 125.6, 125.5, 125.2, 122.9, 122.5, 120.6, 119.14, 119.13, 112.7, 108.3, 30.4.

HRMS (ESI): *m/z* calculated for C<sub>32</sub>H<sub>20</sub>N<sub>2</sub> [M+H]<sup>+</sup>: 433.1705, found [M+H]<sup>+</sup>: 433.1710.

### 5,5'-dimethyl-5H,5'H-6,6'-bibenzo[*b*]carbazole (MeBBCz)



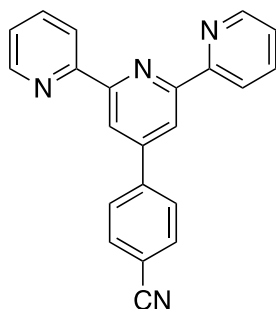
Under argon atmosphere, dibenzocarbazole (*S*)-**8** (122 mg, 0.28 mmol) was dissolved in anhydrous DMF (2 mL) and KO*t*-Bu in *tert*-butanol (1 M) (680 μL, 0.68 mmol) was added dropwise at 0 °C and allowed to stir at RT for 15 minutes. Then, the reaction was cooled to 0 °C and methyl iodide (42 μL, 0.68 mmol) was added dropwise. The reaction mixture was allowed to stir at RT for 1 h before DMF removed under vacuum. The crude product was dissolved using ethylacetate (20 mL) and washed with water (3 X 10 mL) and brine solution (1 x 10 mL). The resulting organic layer was dried over anhydrous Na<sub>2</sub>SO<sub>4</sub> and concentrated under vacuum. The crude product was purified by silica gel column chromatography using 10-15% DCM in n-heptane solvents mixture. The desired compound (*S*)-**5** was obtained as a pale-yellow solid (55.0 mg, 43% yield). The (*R*)-enantiomer was also prepared by using this procedure (69% yield).

<sup>1</sup>H NMR (400 MHz, CDCl<sub>3</sub>) δ 8.81 (s, 2H), 8.34 (d, *J* = 7.7 Hz, 2H), 8.17 (d, *J* = 8.3 Hz, 2H), 7.52 (t, *J* = 7.7 Hz, 2H), 7.40 (dd, *J* = 8.0, 6.8 Hz, 2H), 7.33-7.30 (m, 4H), 7.24 – 7.16 (m, 4H), 2.91 (s, 6H).

<sup>13</sup>C NMR (400 MHz, CDCl<sub>3</sub>) δ 144.3, 140.0, 133.7, 128.5, 127.8, 127.3, 125.6, 125.5, 125.2, 122.9, 122.5, 120.6, 119.1, 112.7, 108.3, 30.4.

HRMS (ESI): *m/z* calculated for C<sub>34</sub>H<sub>24</sub>N<sub>2</sub> [M+H]<sup>+</sup>: 461.2018, found [M+H]<sup>+</sup>: 461.2022.

## CNterpy



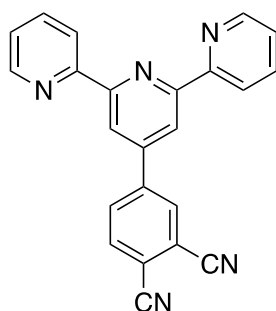
In a dried Schlenck, 4'-Bromo-2,2':6',2''-terpyridine (0.5 g, 2.1 mmol), 4-cyanophenyl boronic acid (0.38 g, 2.55 mmol) and  $K_2CO_3$  (1.95 g, 14 mmol) were dissolved in 21 ml of DMF and 7 ml of water and stirred under Argon. The mixture was bubbling with argon for 15 minutes and before  $Pd(PPh_3)_4$  (0.25 g, 0.2 mmol) was added into a solution, which was refluxed overnight. The reaction was poured into 20 mL of water and the organic layer was extracted 3 times with dichloromethane (3\*20 mL) and thus washed with brine (20 mL) and dried over  $MgSO_4$ . Solvents were removed under vacuum and the product was purified by chromatography (EtOAc/heptane, 50:50) to give the desired product as a white powder in 93% of yield.

$^1H$  NMR (400 MHz,  $CD_2Cl_2$ )  $\delta$  8.79 (s, 2H), 8.77 – 8.61 (m, 4H), 8.02 (d,  $J = 8.5$  Hz, 2H), 7.95 (d,  $J = 7.7$  Hz, 2H), 7.87 (d,  $J = 8.5$  Hz, 2H), 7.43 (t, 2H).

$^{13}C$  NMR (400 MHz,  $CD_2Cl_2$ )  $\delta$  156.0, 149.1, 148.2, 143.0, 136.9, 132.7, 128.0, 124.1, 121.1, 118.7, 112.6.

HRMS (ESI) Maxis 4G, ASAP, 140 °C;  $[M+H]^+$   $m/z$  calculated for  $C_{22}H_{15}N_4$ : 335.12912, found: 335.1294.

## BisCNterpy



In a dried Schlenck, 4'-Bromo-2,2':6',2''-terpyridine borolane (0.31 g, 0.86 mmol), 4-iodophthalonitrile (0.2 g, 0.78 mmol) and  $K_2CO_3$  (0.7 g, 5.2 mmol) were dissolved in 18 mL of DMF and 6 ml of water and stirred under Argon. The mixture was bubbling with argon for 15 minutes before  $Pd(PPh_3)_4$  (0.09 g, 0.08 mmol) was added into the solution, which was

refluxed overnight. The reaction was poured into 20 mL of water and the organic layer was extracted 3 times with dichloromethane (3\*20 mL) and thus washed with brine (20 mL) and dried over MgSO<sub>4</sub>. Solvents were removed under vacuum and the product was purified by chromatography (EtOAc/heptane, 50:50) to give the desired product as a white powder in 88% of yield.

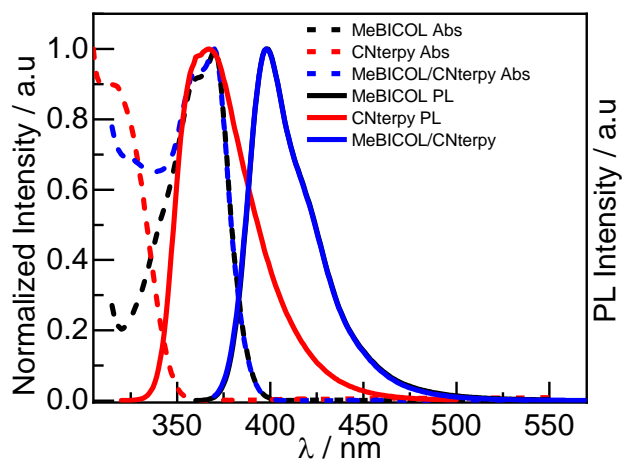
<sup>1</sup>H NMR (400 MHz, CD<sub>2</sub>Cl<sub>2</sub>) δ 8.81 (s, 2H), 8.79 – 8.61 (m, 4H), 8.37 (d, *J* = 1.8 Hz, 1H), 8.28 (dd, *J* = 8.2 Hz, 1H), 8.03 (d, *J* = 8.2 Hz, 1H), 7.97 (t, 2H), 7.45 (t, 2H).

<sup>13</sup>C NMR (400 MHz, CD<sub>2</sub>Cl<sub>2</sub>) δ 156.7, 155.2, 149.2, 146.1, 144.0, 137.0, 134.1, 132.3, 131.8, 124.3, 121.1, 118.5, 116.6, 115.9, 114.9.

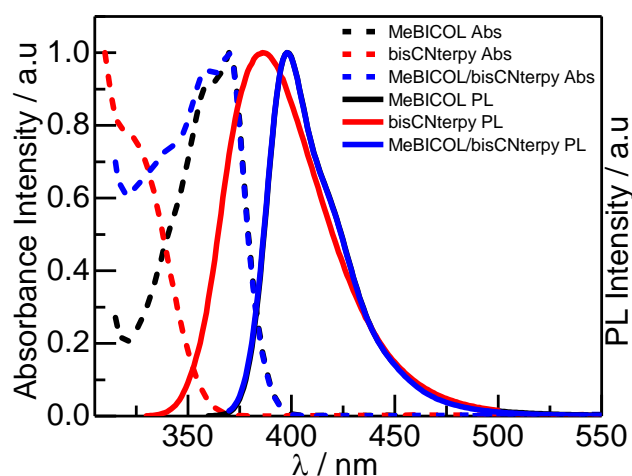
HRMS (ESI) Maxis 4G, ASAP, 150 °C; [M+H]<sup>+</sup> *m/z* calculated for C<sub>23</sub>H<sub>14</sub>N<sub>5</sub>: 360.12437, found: 360.1243.



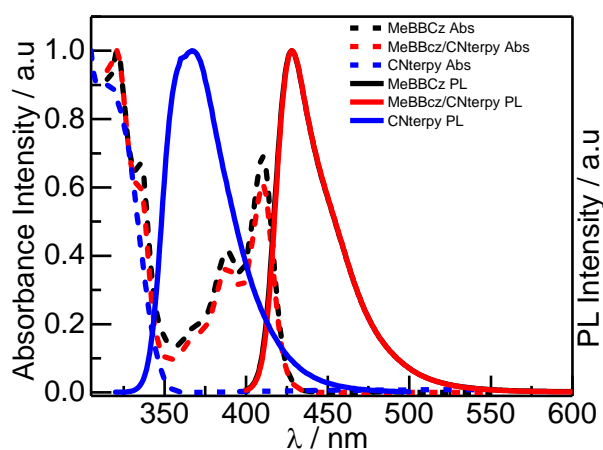
## D. Steady-state photophysical and chiroptical characterizations



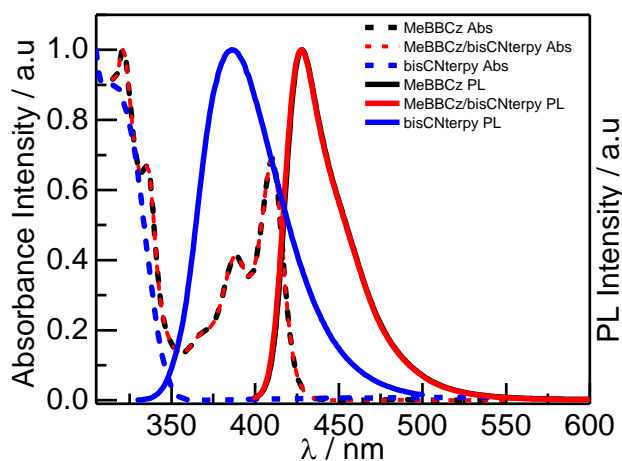
**Figure S1.** Absorption (short dash) and emission (solid) spectra of **MeBICOL** (black), **CNterpy** (red) and a mixture of **MeBICOL/CNterpy** (ratio 2/1) (blue) in DCM (ca.  $10^{-3}$  M).



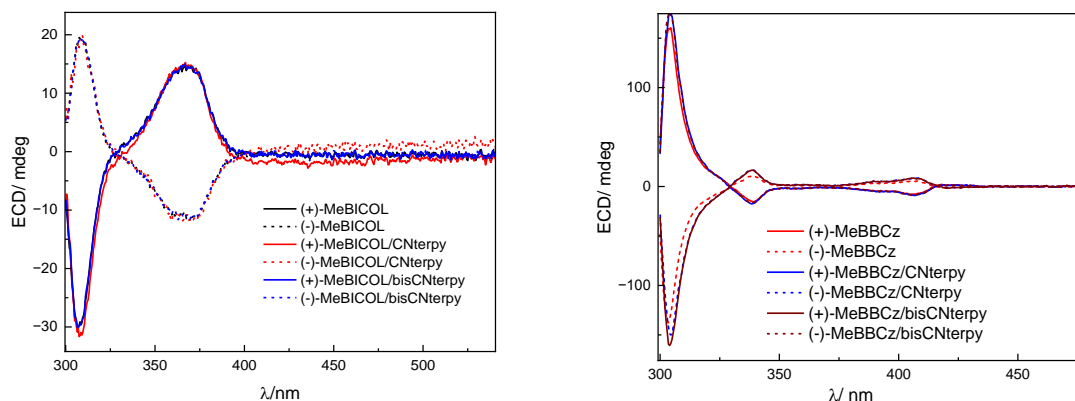
**Figure S2.** Absorption (short dash) and emission (solid) spectra of **MeBICOL** (black), **bisCNterpy** (red) and a mixture of **MeBICOL/bisCNterpy** (ratio 2:1) (blue) in DCM (ca.  $10^{-3}$  M).



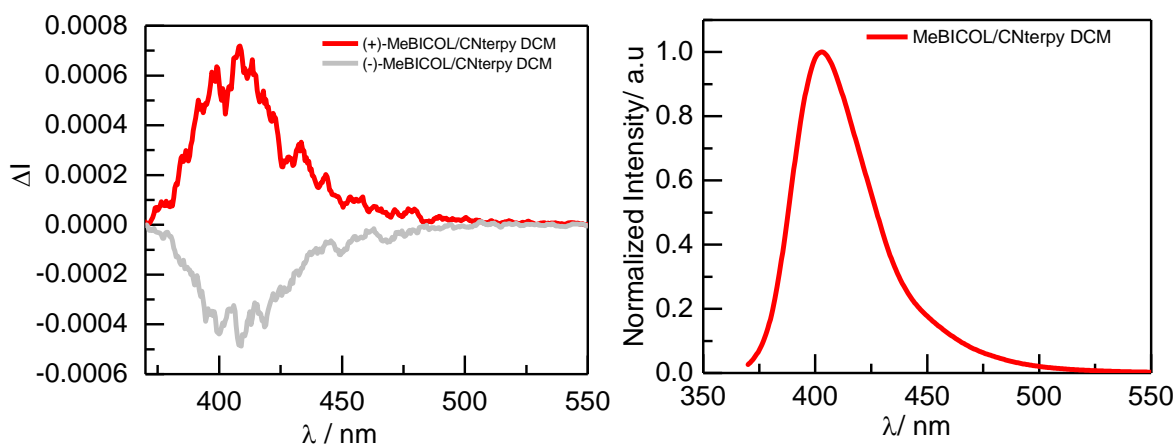
**Figure S3.** Absorption (short dash) and emission (solid) spectra of **MeBBCz** (black), **CNterpy** (blue) and a mixture of **MeBBCz/CNterpy** (ratio 2/1) (red) in DCM (ca.  $10^{-3}$  M).



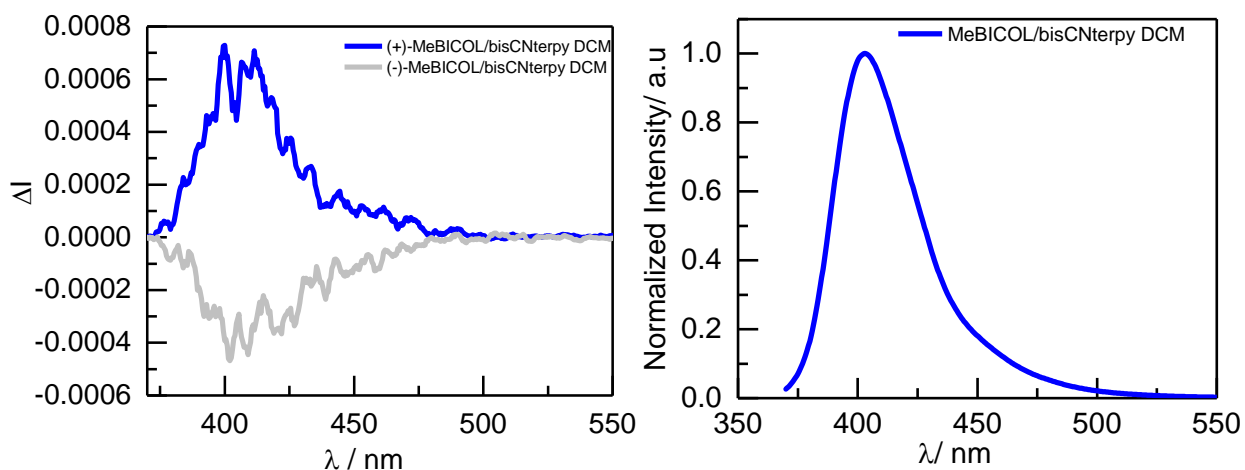
**Figure S4.** Absorption (short dash) and emission (solid) spectra of **MeBBCz** (black), **bisCNterpy** (blue) and a mixture of **MeBBCz/bisCNterpy** (ratio 2/1) (red) in DCM (ca.  $10^{-3}$  M).



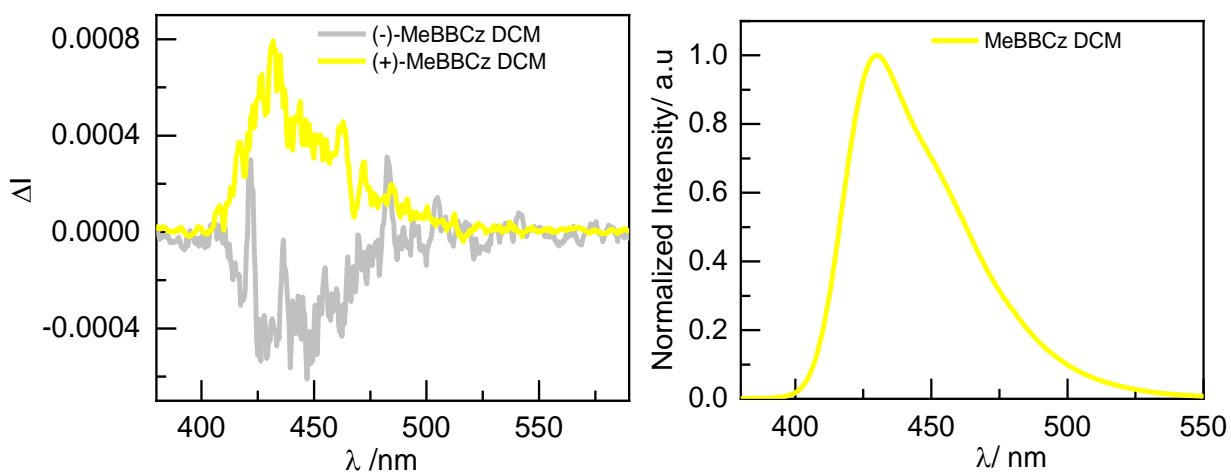
**Figure S5.** Circular dichroism spectra of a mixture of **MeBICOL/CNterpy** and **MeBICOL/CNterpy** (left), and **MeBBCz/CNterpy** and **MeBBCz/CNterpy** (right) spin-coated in glass substrates.



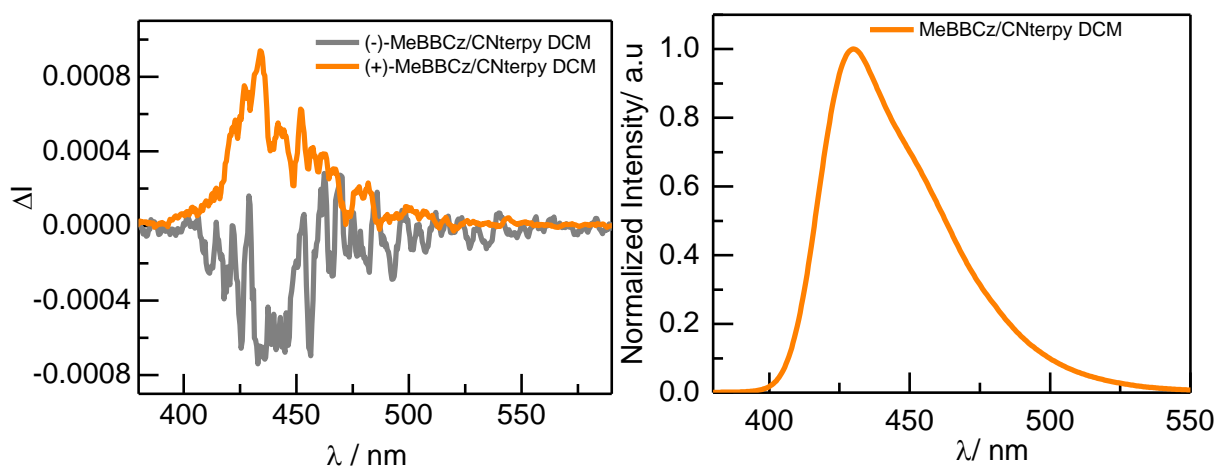
**Figure S6.** CPL and fluorescence spectra of a mixture of **MeBICOL/ CNterpy** (ratio 2:1) in DCM ( $\sim 10^{-5}$  M) at 298 K.



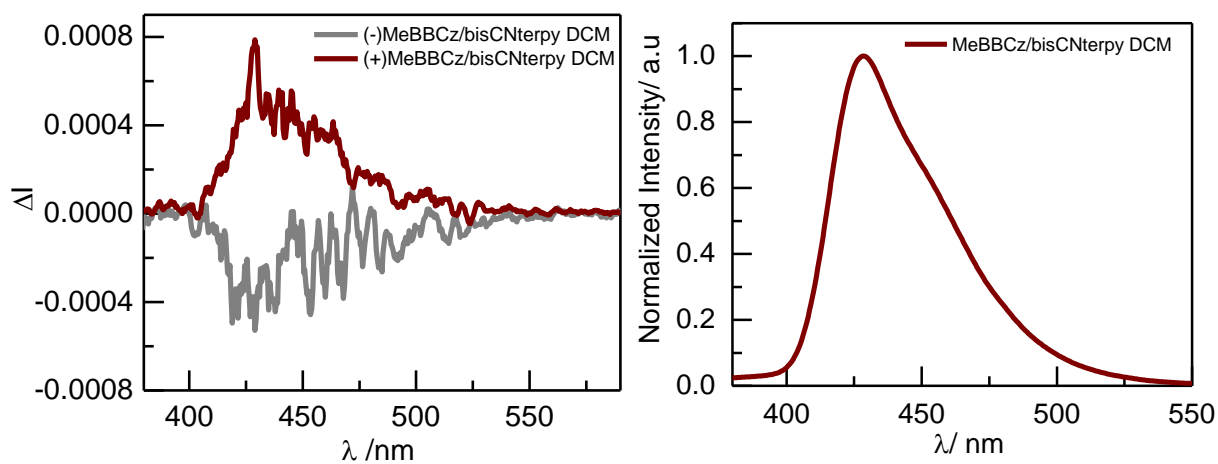
**Figure S7.** CPL and fluorescence spectra of a mixture of **MeBICOL/bisCNterpy** (ratio 2:1) in DCM ( $\sim 10^{-5}$  M) at 298 K.



**Figure S8.** CPL and fluorescence spectra of donor **MeBBCz** in DCM ( $\sim 10^{-5}$  M) at 298 K.

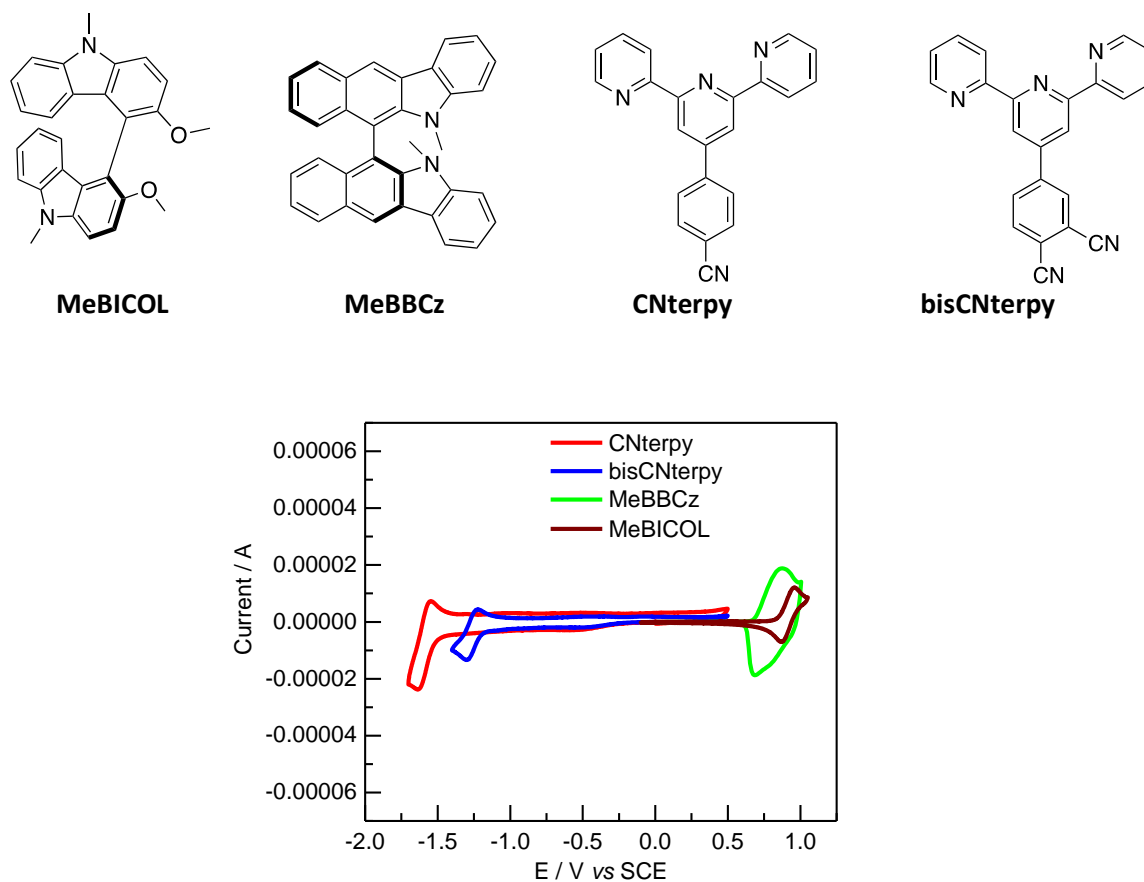


**Figure S9.** CPL and fluorescence spectra of a mixture of **MeBBCz/CNterpy** (ratio 2:1) in DCM ( $\sim 10^{-5}$  M) at 298 K.

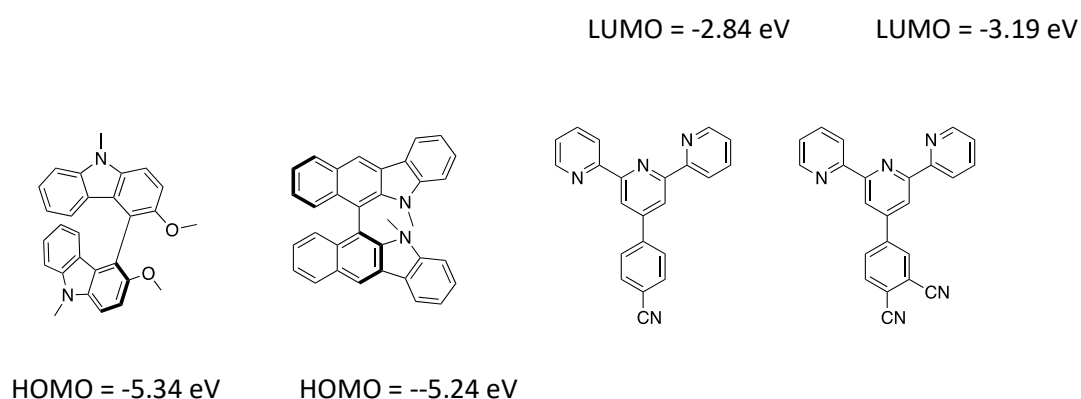


**Figure S10.** CPL and fluorescence spectra of a mixture of **MeBBCz/bisCNterpy** (ratio 2:1) in DCM ( $\sim 10^{-5}$  M) at 298 K.

## F. Exciplex Characterizations



**Figure S11.** Cyclic voltammograms of donor and acceptor compounds versus saturated calomel electrode (SCE) as the reference and 0.2 M  $\text{Bu}_4\text{NPF}_6$  in  $\text{CH}_2\text{Cl}_2$  with a scan rate of 200 mV/s.



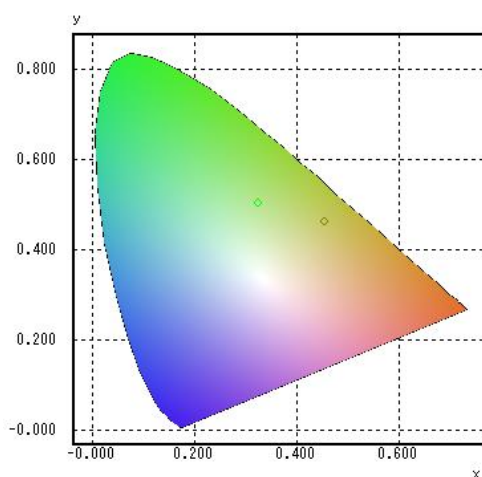
**Figure S12.** Chemical structures of the different electron donor and acceptors screened in this study to obtain multi-colored chiral exciplex luminescence with their HOMO and LUMO values, estimated from their oxidation and reduction potentials (assuming a value of -4.44 eV for 0 V vs SCE).

**Table S1.** HOMO and LUMO energy levels (in eV) of chiral donor and achiral acceptor units

Compounds	HOMO [a]	LUMO [b]
<b>MeBICOL</b>	-5.34	
<b>MeBBCz</b>	-5.24	
<b>CNterpy</b>		-2.84
<b>bisCNterpy</b>		-3.19

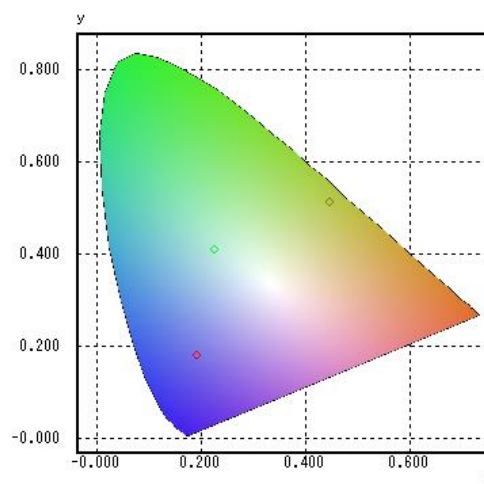
[a] HOMO= $-(4.44+E_{ox}^{onset})$

[b] LUMO= $-(4.44+E_{re}^{onset})$



a)

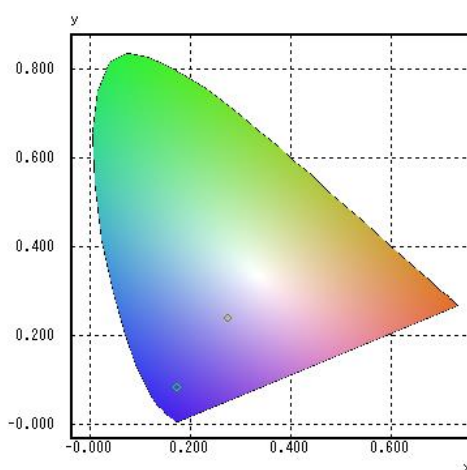
**MeBICOL/CNterpy and MeBICOL/bisCNterpy**



b)

**MeBBCz, MeBBCz/CNterpy and MeBBCz/bisCNterpy**

c)

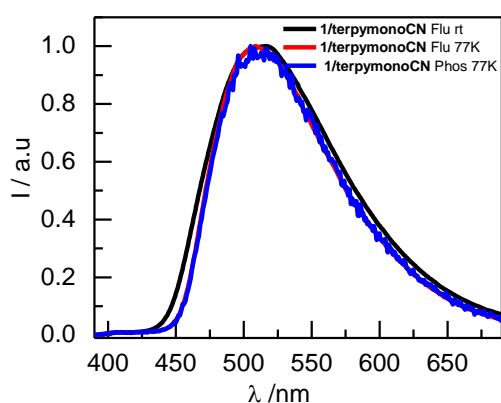


**CNterpy and bisCNterpy**

**Figure S13.** CIE diagrams obtained from the emissions of a) **MeBICOL/CNterpy** and **MeBICOL/bisCNterpy** exciplexes, b) **MeBBCz** alone, **MeBBCz/CNterpy** and **MeBBCz/bisCNterpy** exciplexes, c) **CNterpy** and **bisCNterpy** alone, obtained from spin-coated film at 298 K.

**Table S2.** Fluorescence quantum yields ( $\Phi_{PL}$ ) of exciplexes involving **MeBICOL**, **MeBBCz**, **CNterpy** and **bisCNterpy** (ratio 2:1) on films under air atmosphere.

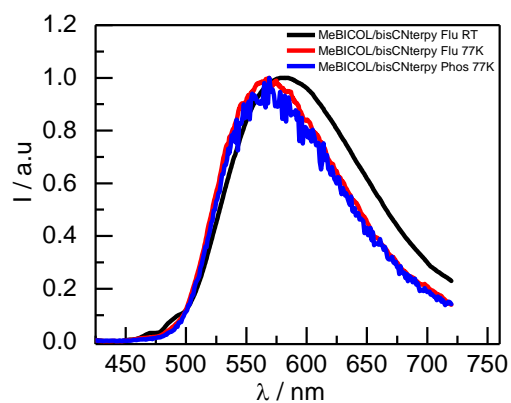
Compounds	$\Phi_{PL}$ (%)	
	Air	vacuum
<b>MeBICOL</b>	5.9	n.d.
<b>MeBBCz</b>	8	n.d.
<b>MeBICOL/CNterpy</b>	8	11
<b>MeBICOL/bisCNterpy</b>	2	7
<b>MeBBCz/CNterpy</b>	10	19
<b>MeBBCz/bisCNterpy</b>	10	19
<b>CNterpy</b>	10	n.d.
<b>bisCNterpy</b>	8	n.d.



$$S_1 = 1240/435 = 2.85 \text{ eV}$$

$$T_1 = 1240/448 = 2.77 \text{ eV}$$

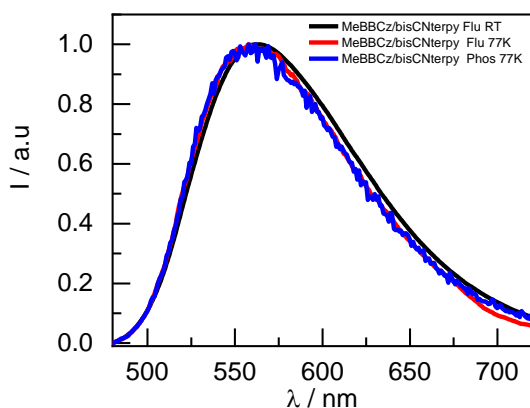
$$\Delta E(ST) = \sim 0.08 \text{ eV}$$



$$S_1 = 1240/498 = 2.49 \text{ eV}$$

$$T_1 = 1240/485 = 2.49 \text{ eV}$$

$$\Delta E(ST) = \sim 0.01 \text{ eV}$$

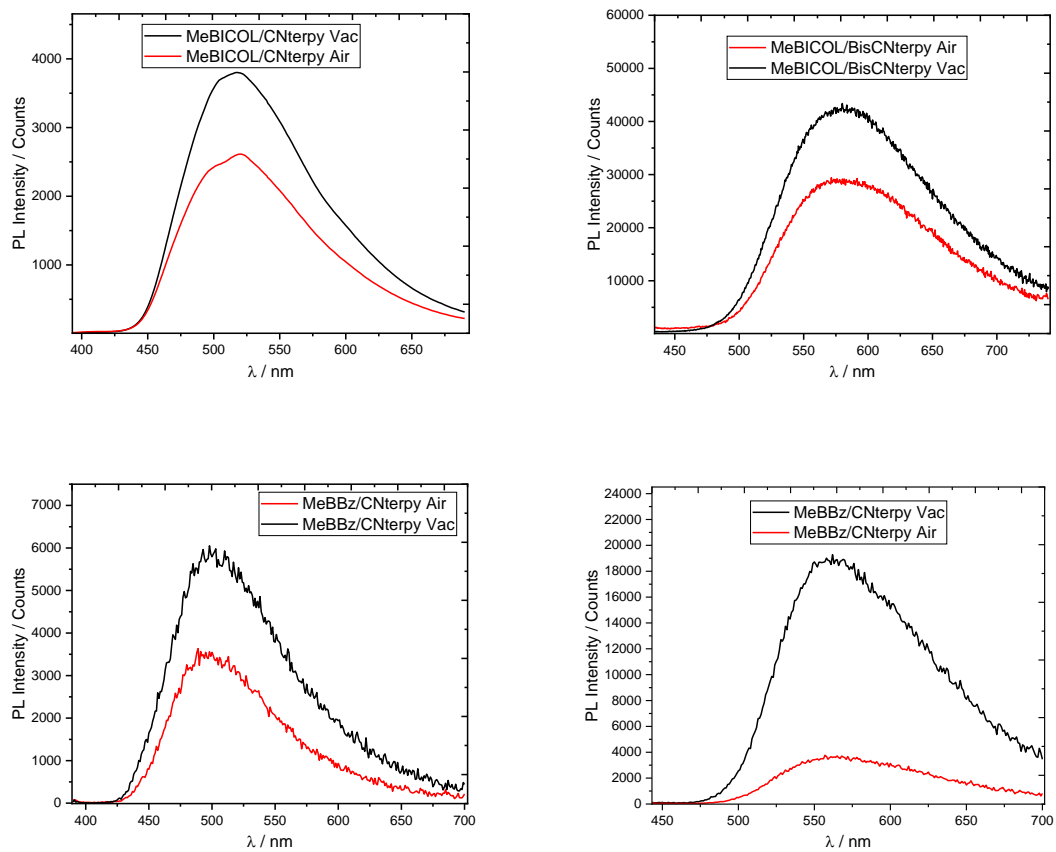


$$S_1 = 1240/498 = 2.49$$

$$T_1 = 1240/499 = 2.49$$

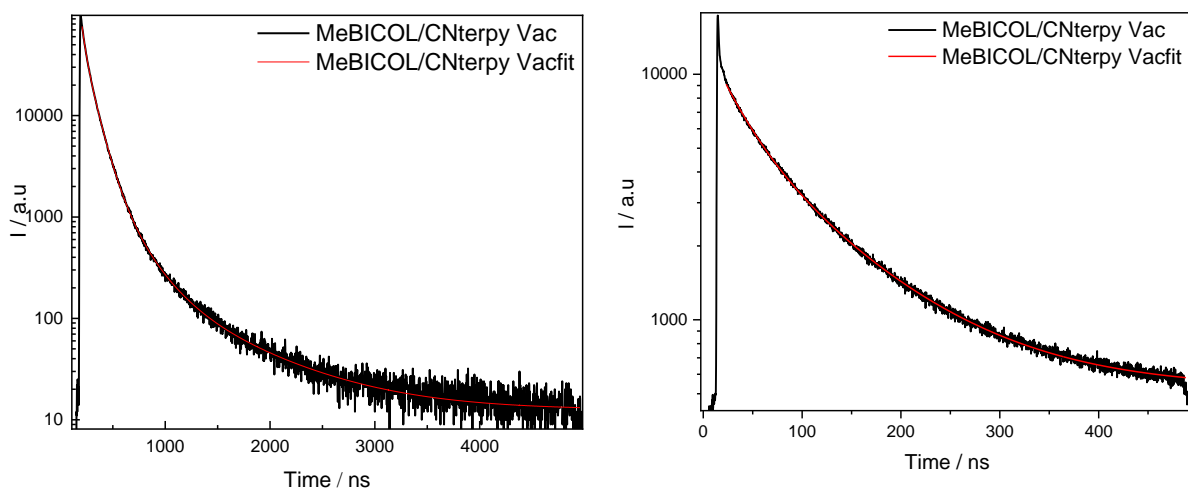
$$\Delta E(ST) = \sim 0.01 \text{ eV}$$

**Figure S14.** Luminescence spectra of **MeBICOL/CNterpy** (top left), **MeBICOL/bisCNterpy** (top right), and of **MeBBCz/bisCNterpy** exciplex (bottom), at RT (black), 77 K (red) and gated at 77 K in neat films (excited 370 nm, delayed 20 ms).

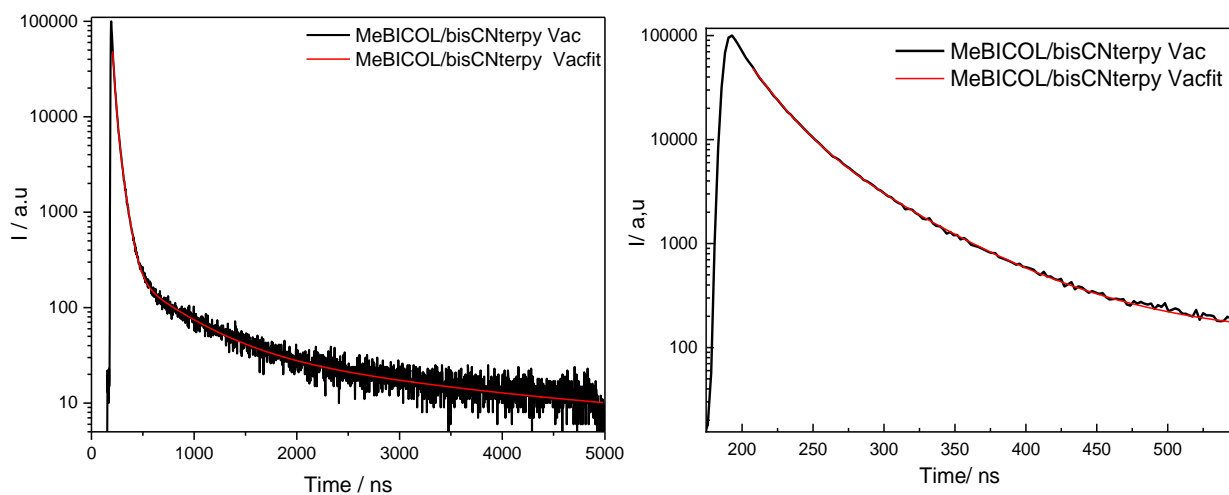


**Figure S15.** Emission spectra of exciplexes **MeBICOL/CNterpy** and **MeBICOL/bisCNterpy** (top), and **MeBBz/CNterpy** and **MeBBz/bisCNterpy** (bottom) in neat films under vacuum (black) and air (red) conditions.

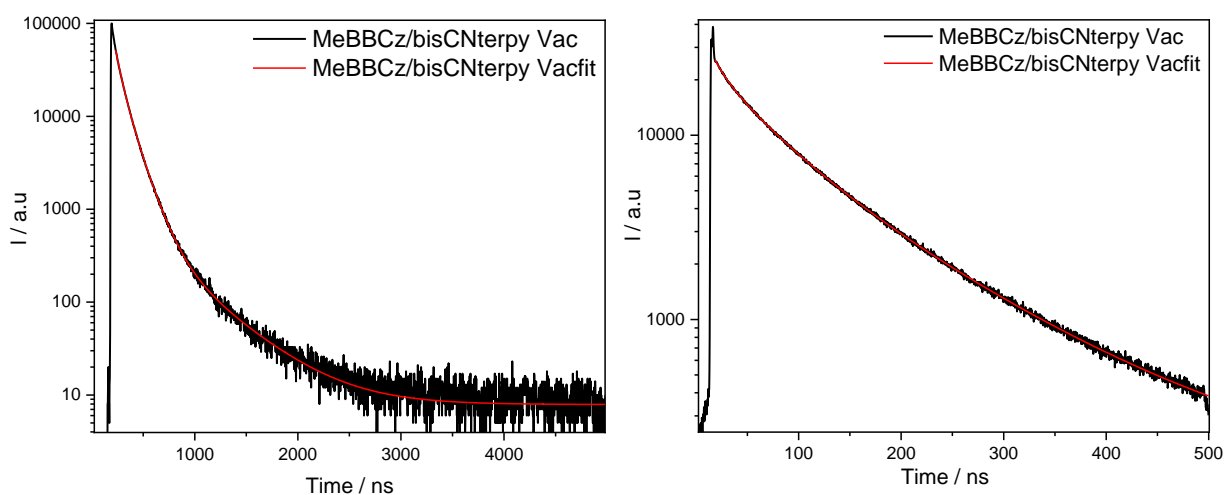




**Figure S16.** Luminescence decay of **MeBICOL/CNterpy** (ratio 2:1) in solid state at 298 K and under vacuum (back) with corresponding red fits for the microseconds, monitored at 510 nm.



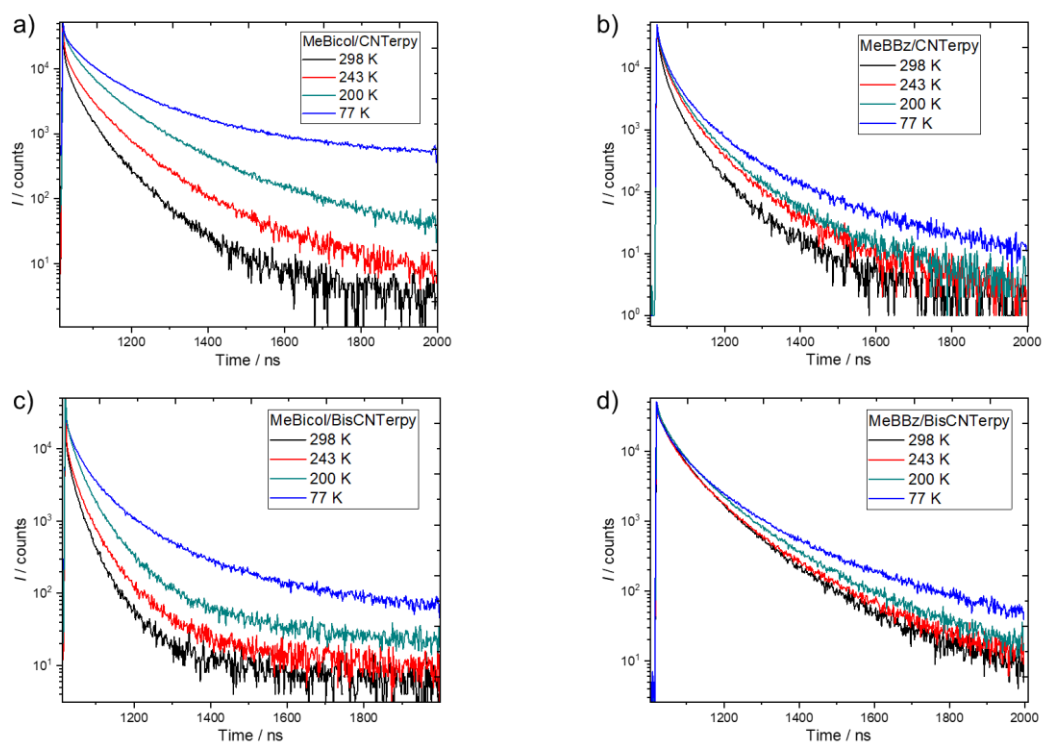
**Figure S17.** Luminescence decay of **MeBICOL/bisCNterpy** (ratio 2:1) in solid state at 298 K and under vacuum (black) with corresponding red fits for the microseconds, monitored at 550 nm.



**Figure S18.** Luminescence decay of **MeBBCz/bisCNterpy** (ratio 2:1) in solid state at 298 K and under vacuum (black) with corresponding red fits for the microseconds, monitored at 550 nm.

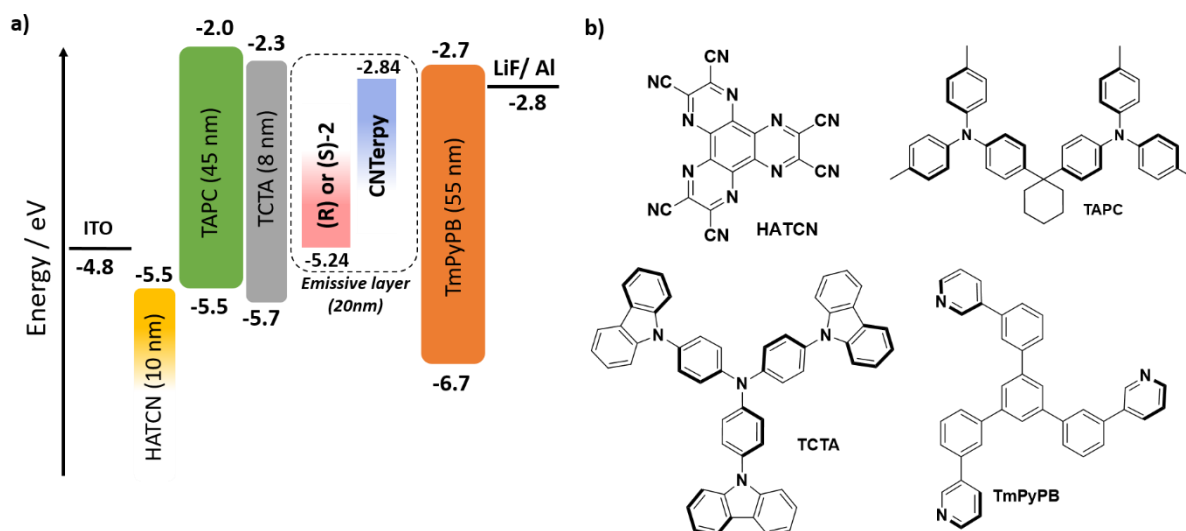
**Table S3.** Photophysical and chiroptical properties of exciplex emitters.

Compounds	$\lambda_{\text{abs}}$ (nm)	$\lambda_{\text{em}}$ (nm)		$T_{\text{pf \& df}}$		$\Delta E_{\text{ST}}$ (eV)	$g_{\text{lum}}$ ( $10^{-3}$ )	
		DCM	Film	(ns)	(ns)		DCM	Films
<b>MeBICOL/CNterpy</b>	370	398	512	57.4 131.3	560.1	0.08	0.5	7
<b>MeBICOL/bisCNterpy</b>	370	398	581	19.6 56.3	706.4	0.01	0.5	4
<b>MeBBCz/CNterpy</b>	409	426	492	37.7 81.3	493.7	0.04	0.7	10
<b>MeBBCz/bisCNterpy</b>	409	426	562	53.9 122.8	453.2	0.06	0.6	2



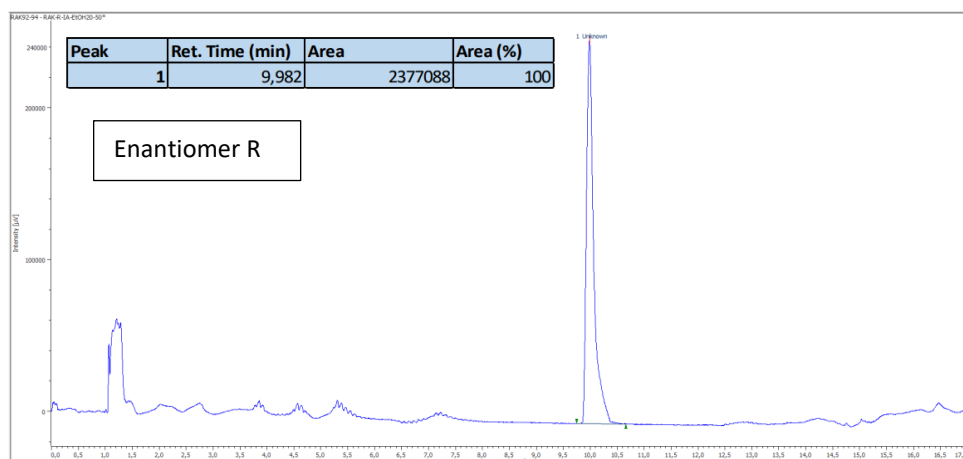
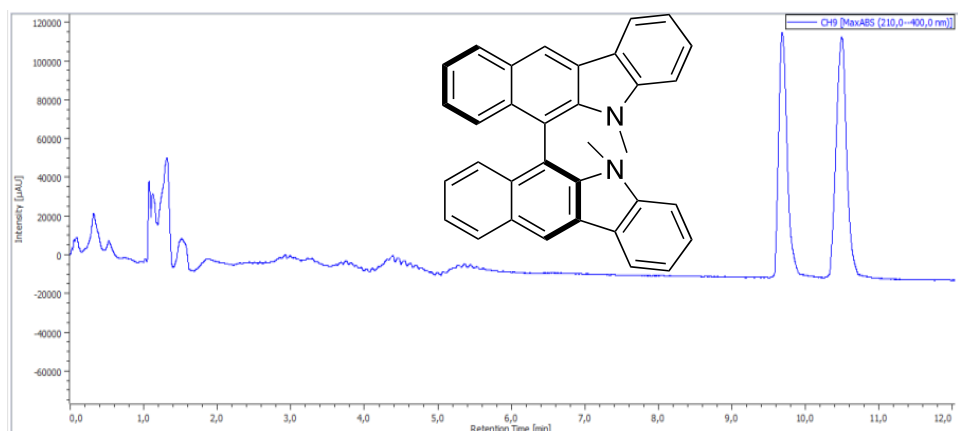
**Figure S19.** Luminescence decay of exciplexes a) **MeBicol/CNterpy** and b) **MeBBz/CNterpy** (top), c) **MeBicol/BisCNterpy** and d) **MeBBz/bisCNterpy** (bottom) in neat films at 77 K (blue), 200 K (green), 243 K (red) and 298 K (black).

## E. OLED fabrication



**Figure S20.** Energy level diagram of the OLED architecture with the chemical structures of the compounds used for the different layers.

## F. HPLC separation



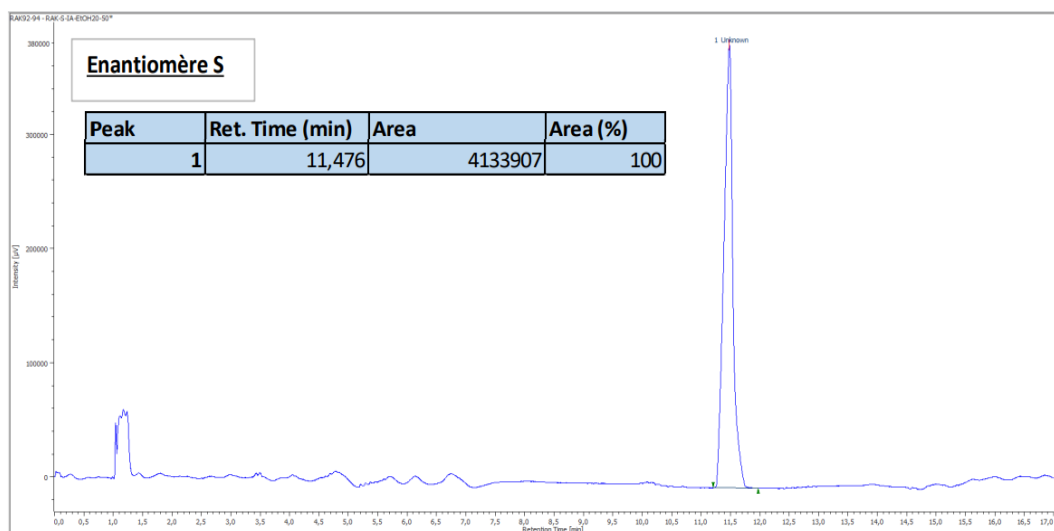


Figure S21. Chiral HPLC of MeBBCz.

## F. NMR spectra

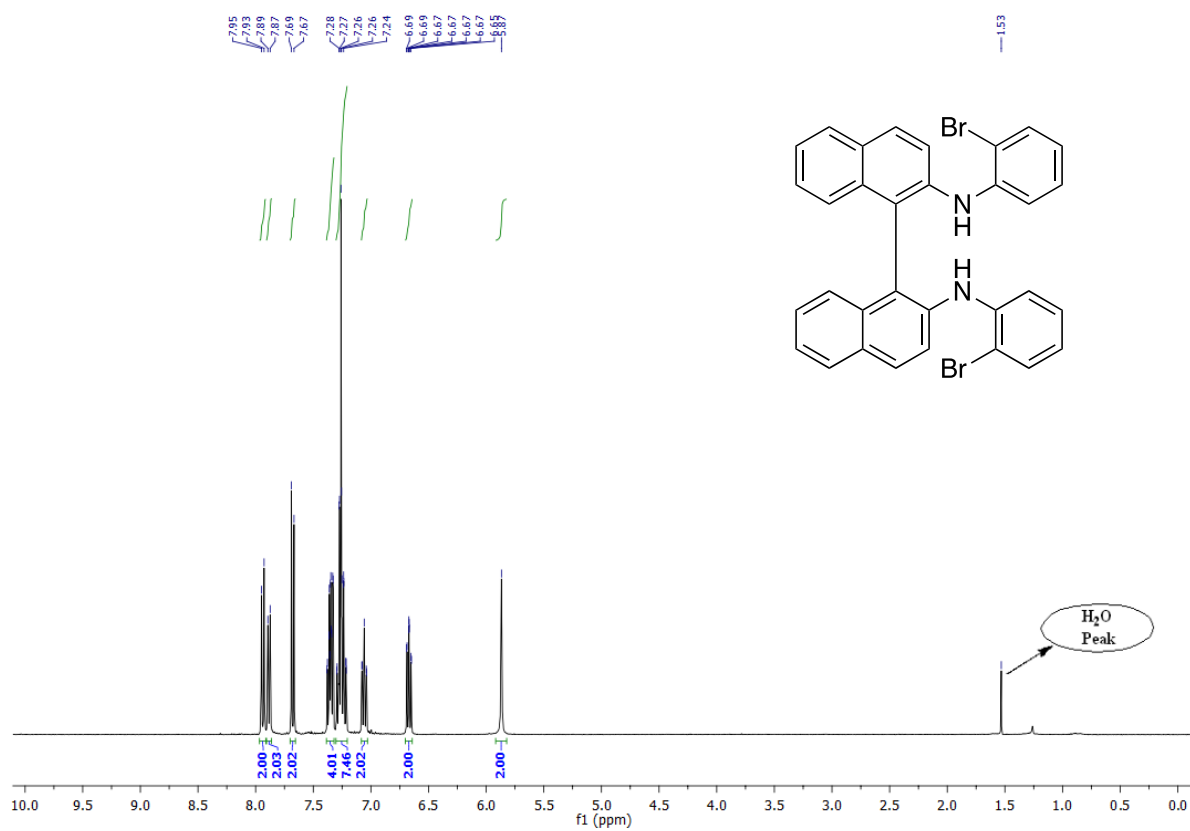


Figure S22. <sup>1</sup>H-NMR spectra of 7 in CDCl<sub>3</sub>.

100.47  
138.53  
138.52  
132.28  
129.86  
128.29  
127.91  
124.64  
124.12  
124.12  
119.10  
118.79  
117.16  
113.80

77.32  
76.86  
76.88

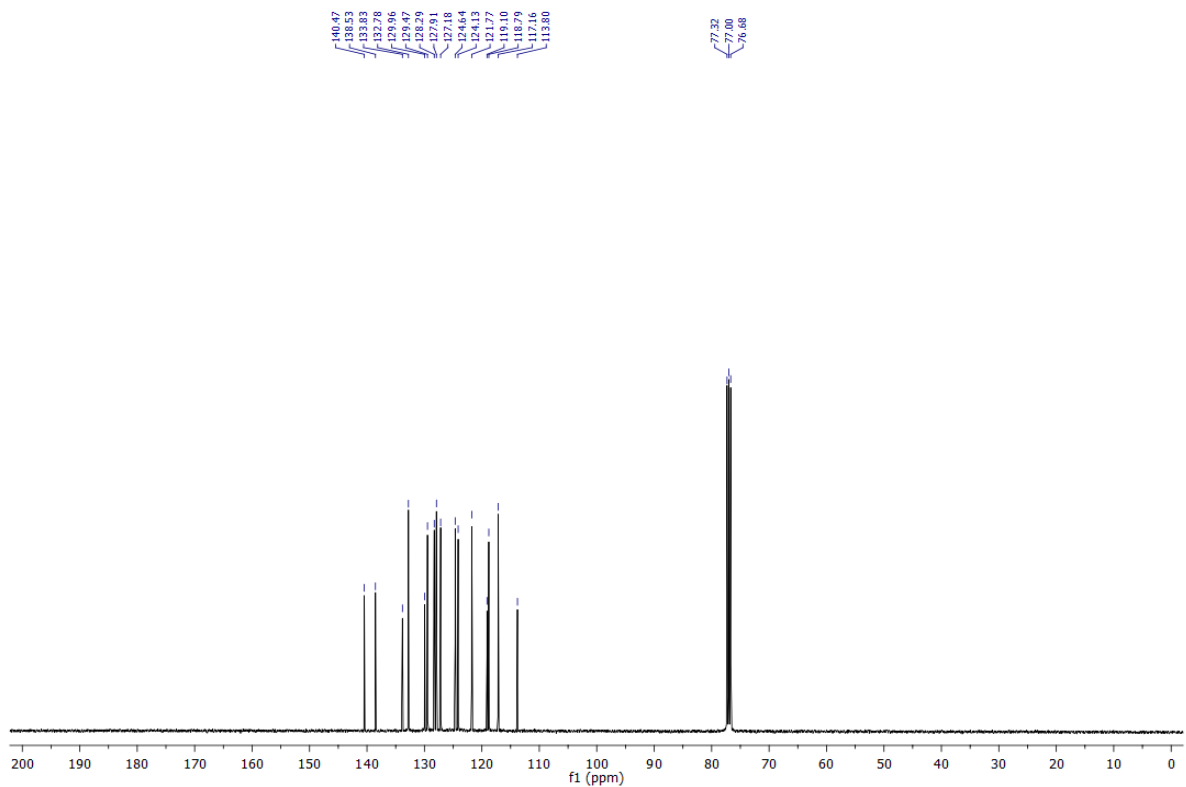


Figure S23.  $^{13}\text{C}$ -NMR spectra of **7** in  $\text{CDCl}_3$ .

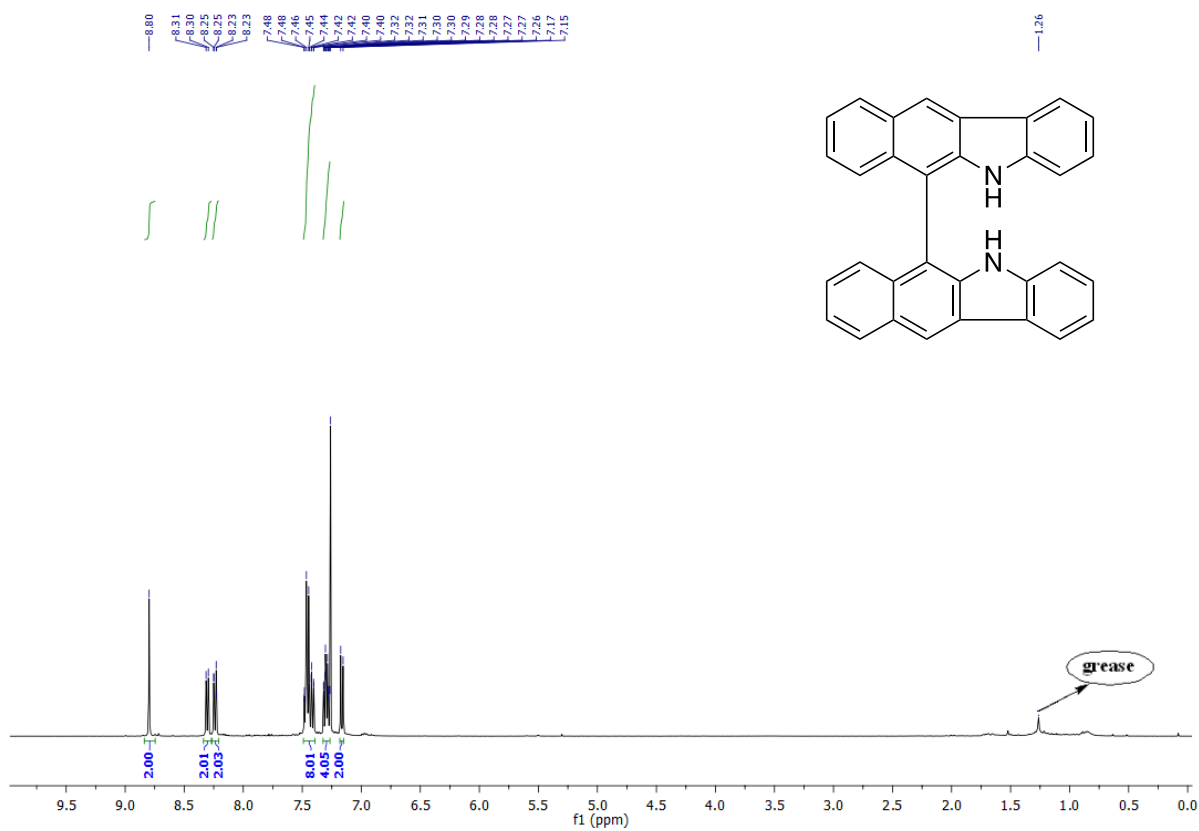


Figure S24.  $^1\text{H}$ -NMR spectra of **8** in  $\text{CDCl}_3$ .

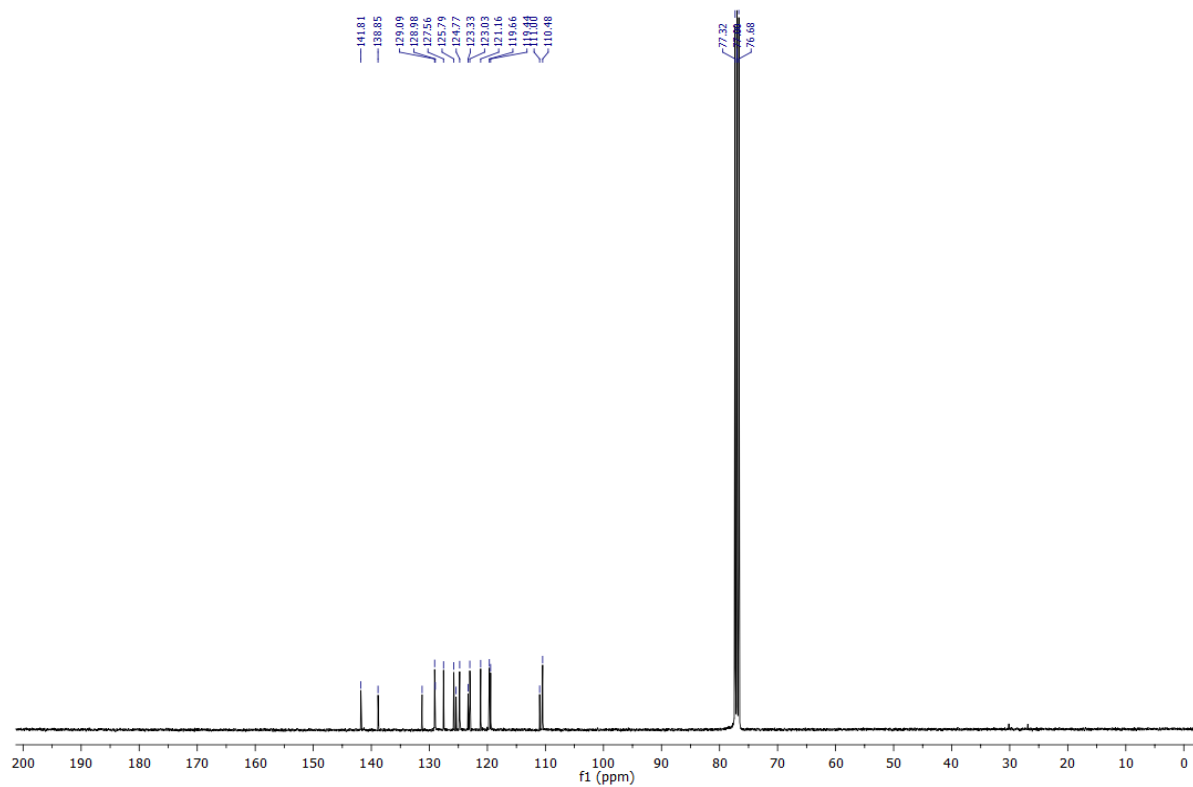


Figure S25.  $^{13}\text{C}$ -NMR spectra of **8** in  $\text{CDCl}_3$ .

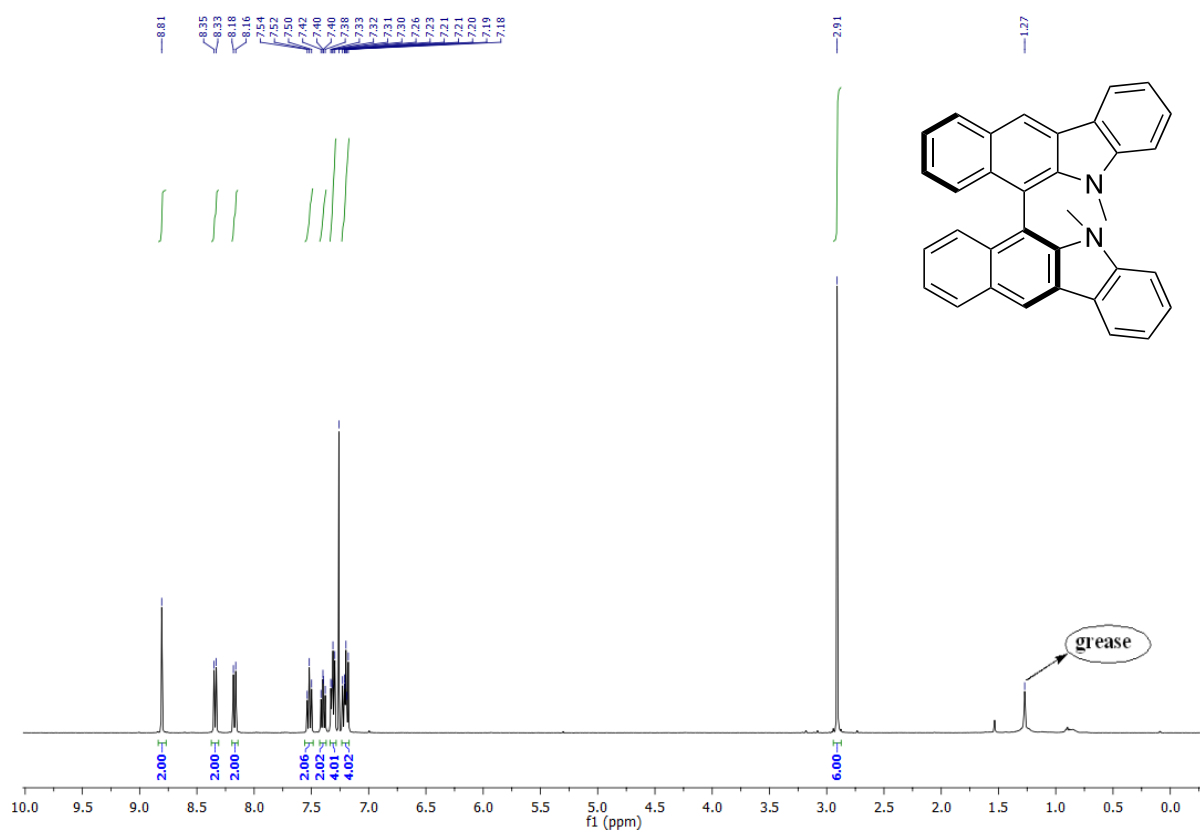


Figure S26.  $^1\text{H}$ -NMR spectra of **MeBBCz** in  $\text{CDCl}_3$ .

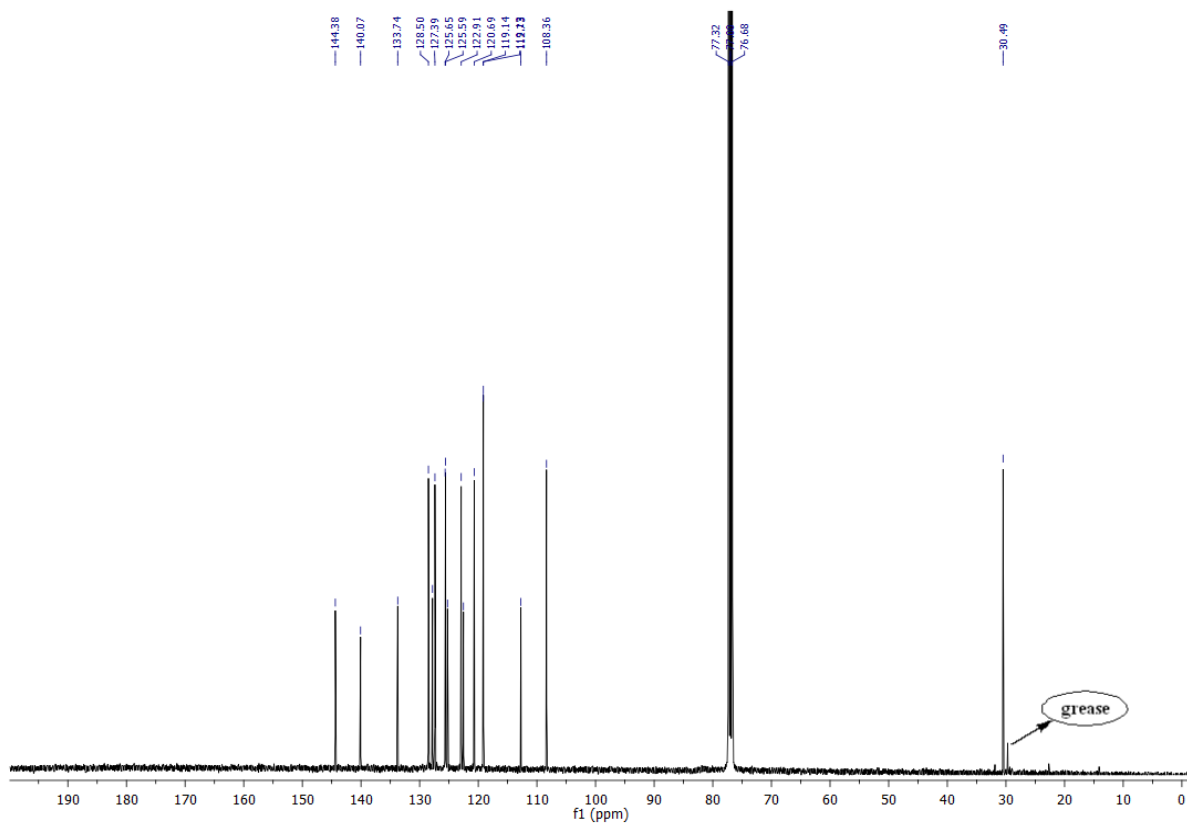


Figure S27.  $^{13}\text{C}$ -NMR spectra of MeBBCz in  $\text{CDCl}_3$ .

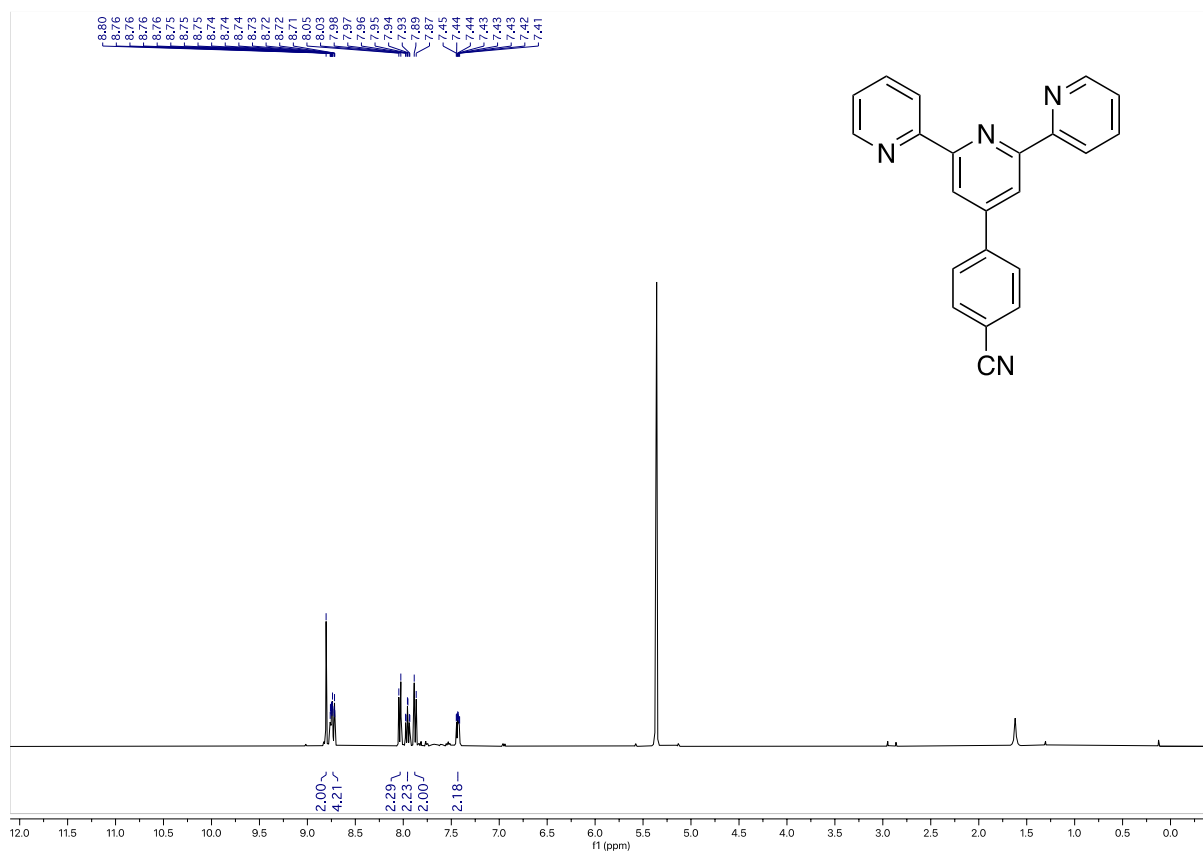


Figure S28.  $^1\text{H}$ -NMR spectra of CNterpy in  $\text{CD}_2\text{Cl}_2$ .



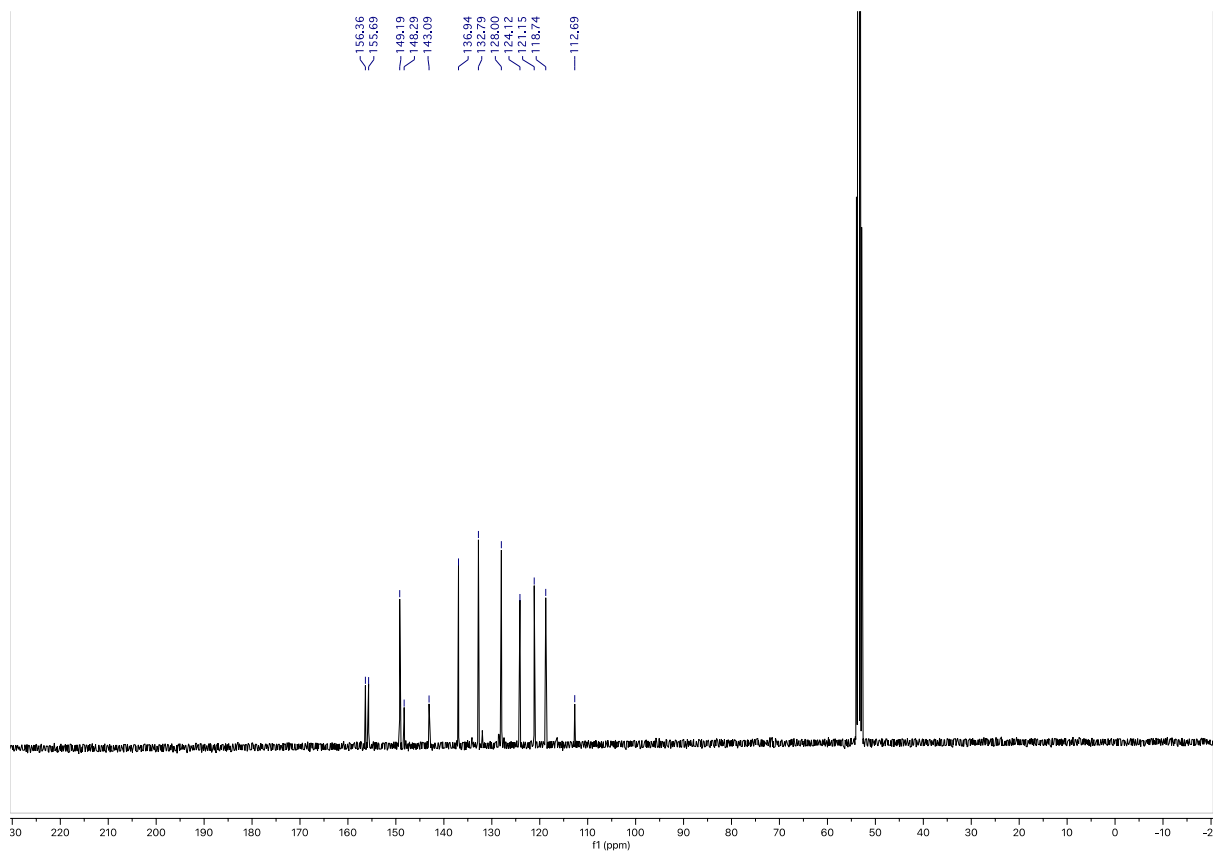


Figure S29.  $^{13}\text{C}$ -NMR spectra of **CNterpy** in  $\text{CD}_2\text{Cl}_2$ .

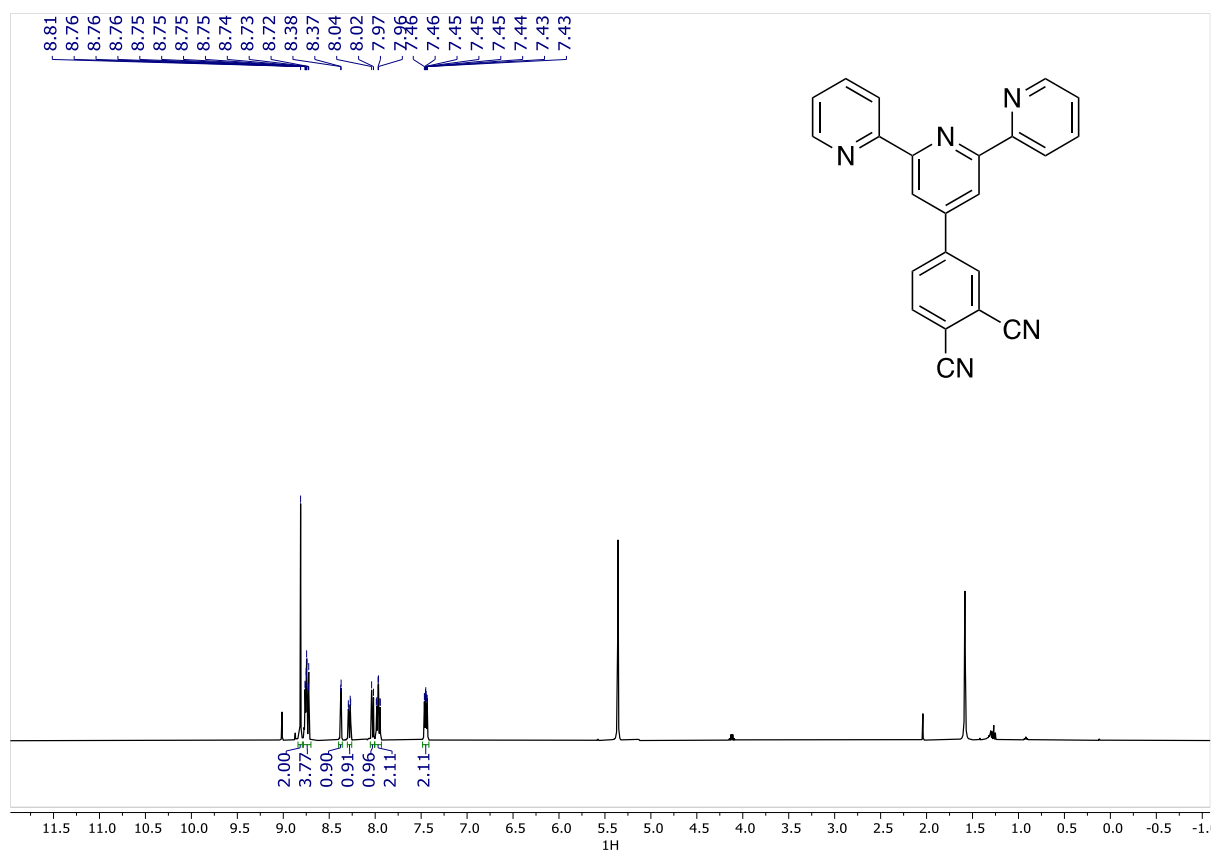


Figure S30.  $^1\text{H}$ -NMR spectra of **bisCNterpy** in  $\text{CD}_2\text{Cl}_2$ .

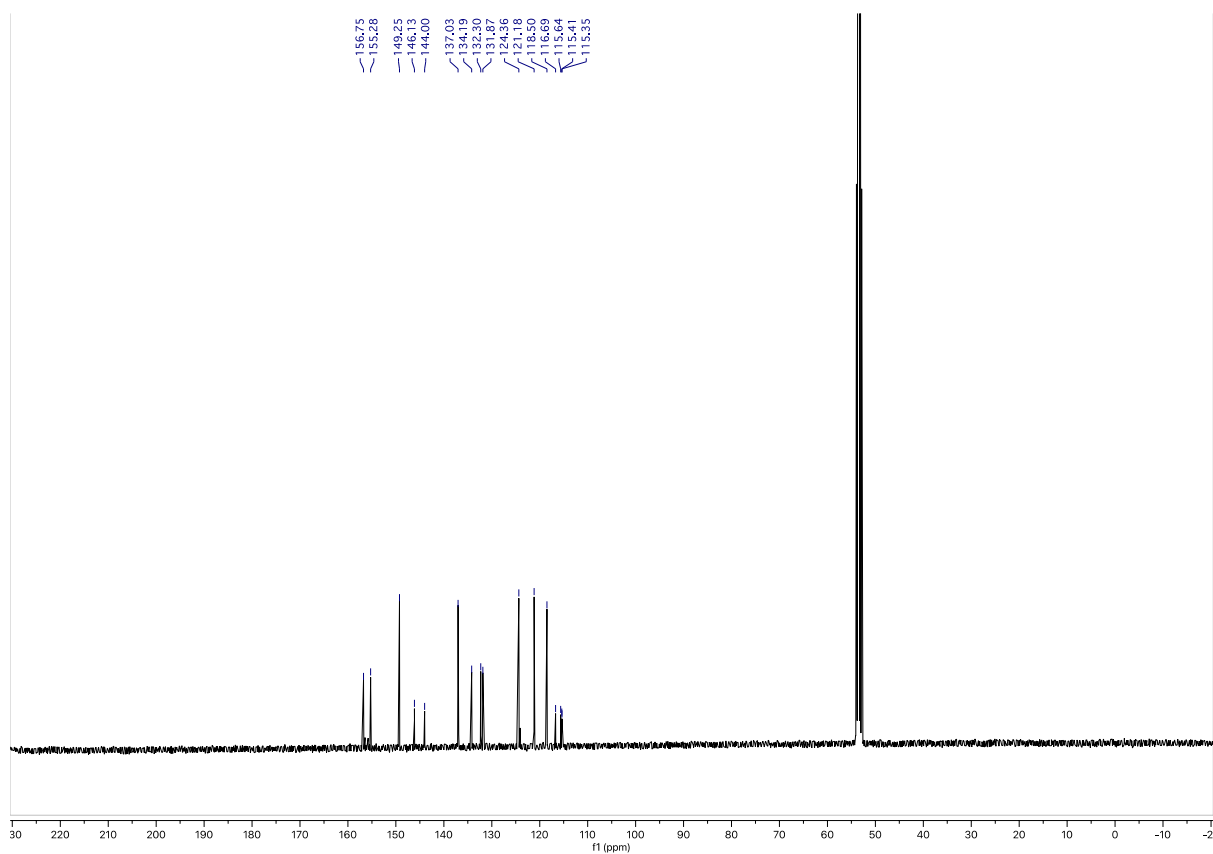


Figure S31.  $^{13}\text{C}$ -NMR spectra of bisCNterpy in  $\text{CH}_2\text{Cl}_2$ .