Supporting Information

# Multiple-resonant nitrogen embedded nanographenes with high photoluminesence efficiency and high colour purity

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## General Procedures

All reagents were purchased from InnoChem Co. (Beijing, China) or Energy Chemicals Co. and used directly without further purification. Unless otherwise mentioned, all the reactions were operated under nitrogen atmosphere and corresponding products were purified through column chromatography. The $^{1}H$/$^{13}C$ NMR spectra were recorded on Bruker Fourier 300 spectrometer and Bruker AVANCE III 400 spectrometer at 298 K. Chemical shifts are reported as δ: values (in ppm) with tetramethylsilane (TMS) as the internal standard. HR-MALDI-TOF mass spectra were collected by an Autoflex III (Bruker Daltonics Inc.) MALDI-TOF spectrometer.

**Theoretical Calculation:** Calculations were carried out as implemented in Gaussian 16 program. The molecular structures were optimized by dispersion corrected denisty functional theory (DFT-D3) at B3LYP-D3/6-31G(d,p) level. [1-4] The solvation model based on density (SMD) implicit solvent model was used to describe the solvent effect of toluene. The molecular geometries at the first excited state ($S_1$) were optimized at the B3LYP-D3/6-31G(d,p) level with the time-dependent density functional theory (TD-DFT) method. Vibrational frequency analysis was carried out for these optimized structures with the same calculation method to obtain the Hessian of the first excited state and vibrational coordinates. The vibration-resolved emission spectra were given by using the Franck-Condon-Herzberg-Teller method[5], broadening with a half width at half-maximum of 300 $cm^{-1}$.

**Electrochemical Analysis**: Electrochemical measurements were carried out on a CHI660c electrochemical workstation with a three-electrode-cell structure with glassy carbon stick electrode as working electrode, platinum wire as auxiliary electrode, and Ag+/Ag electrode as reference electrode. The circular voltammetry (CV) curves were measured in dichloromethane (for oxidative potentials) or tetrahydrofuran (for reductive potentials) containing 0.1 M tetrabutylammonium hexylfluorophosphate as supporting electrolyte standardized against ferrocene/ferrocenium with a scan rate of 100 mV/s.

**X-ray Crystallography:** Diffraction data were collected at 293 K on a Rigaku Saturn 724 CCD diffract meter with graphite monochromated Mo·Kα radiation. The crystallography data was deposited in the Cambridge Crystallographic Data Centre (CCDC) and the CCDC number for the structure was offered.

**Thermogravimetric Analysis:** Thermogravimetric analysis (TGA) was performed on a PerkinElmer series 7 thermal analysis system under the nitrogen atmosphere with a heating rate of 10ºC/min, scanning from 50-700 ºC.

**Photophysical Property Measurement:** UV-vis absorption spectra were measured on a HITACHI UH4150 spectrophotometer. Emission spectra were measured on an Edinburgh FS5 fluorimeter. An Edinburgh FLS980 fluorimeter was employed to record the PL decay curves. The absolute quantum yields of solutions were determined by using a Hiroba FluoroMax+ fluorimeter with an integrating sphere system. The phosphorescent spectra were measured in toluene on an Edinburgh Instruments LP920-KS fluorescence spectraphotometer at 77 K cooled by liquid nitrogen with a delay of 5 ms using the Time-Correlated Single Photon Counting (TCSPC) method with a pulse laser (Vibrant 355II).

## Theoretical Calculation Results

**Table S1** Summary of TD-DFT calculation at B3LYP-D3/6-31G(d,p) level for ICz, ICz-2 and ICz-3 at the optimized $S_0$, $S_1$ and $T_1$ structures in toluene

| Compound | Optimized Structure | Transition | Wavelength [nm] | Energy [eV] | Oscillator Strength |
|---|---|---|---|---|---|
| ICz | $S_0$ | $S_0$-$S_1$ | 340.41 | 3.6433 | 0.1053 |
| | | $S_0$-$T_1$ | 414.47 | 2.9914 | 0 |
| | $S_1$ | $S_1$-$S_0$ | 377.25 | 3.2866 | 0.0291 |
| ICz-2 | $S_0$ | $S_0$-$S_1$ | 433.84 | 2.8578 | 0.4630 |
| | | $S_0$-$T_1$ | 537.21 | 2.3079 | 0 |
| | $S_1$ | $S_1$-$S_0$ | 463.61 | 2.6743 | 0.7105 |
| ICz-3 | $S_0$ | $S_0$-$S_1$ | 499.97 | 2.4798 | 0.5273 |
| | | $S_0$-$T_1$ | 625.01 | 1.9837 | 0 |
| | $S_1$ | $S_1$-$S_0$ | 529.74 | 2.3405 | 0.6202 |

**Table S2** Summary of Franck-Condon analysis at B3LYP-D3/6-31G(d,p) level for ICz, ICz-2 and ICz-3 in toluene

| Compound | Transition No. | Transition Mode | Frequency [cm$^{-1}$] | Relative Frequency [cm$^{-1}$] | Intensity | Dipole Strength |
|---|---|---|---|---|---|---|
| ICz | 1 | $70^1 14^1$ | 24891.5319 | -2161.8881 | 1.590 | 0.004058 |
| | 2 | $70^1 4^1$ | 25256.3194 | -1791.1006 | 2.065 | 0.004971 |
| | 3 | $70^1$ | 25411.2913 | -1642.1287 | 3.376 | 0.007933 |
| | 4 | $14^2$ | 26013.9012 | -1039.5188 | 1.944 | 0.004160 |
| | 5 | $26^1$ | 26295.8195 | -757.6005 | 2.270 | 0.004651 |
| | 6 | $14^1 4^1$ | 26378.6888 | -674.7312 | 5.078 | 0.01028 |
| | 7 | $14^1$ | 26533.6606 | -519.7594 | 8.656 | 0.01711 |
| | 8 | $10^1$ | 26652.0293 | -400.3907 | 2.384 | 0.004628 |
| | 9 | $4^2$ | 26743.2763 | -309.9437 | 4.433 | 0.008491 |
| | 10 | $4^1$ | 26899.4481 | -153.9719 | 12.43 | 0.02327 |
| | 11 | 0 | 27053.4200 | 0 | 20.47 | 0.03745 |
| ICz-2 | 1 | $2^1 1^5$ | 21299.9385 | -63.1404 | 65.90 | 0.1255 |
| | 2 | $2^1 1^4$ | 21310.3327 | -52.7462 | 87.13 | 0.1656 |
| | 3 | $2^1 1^3$ | 21320.7269 | -42.3520 | 87.40 | 0.1658 |
| | 4 | $1^4$ | 21321.5023 | -41.5766 | 60.54 | 0.1148 |
| | 5 | $2^1 1^2$ | 21331.1210 | -31.9579 | 62.63 | 0.1185 |
| | 6 | $1^3$ | 21331.8964 | -31.1825 | 63.05 | 0.1193 |
| | 7 | 0 | 21363.0789 | 0 | 4.999 | 0.009406 |
| ICz-3 | 1 | $5^1 1^2$ | 18444.2507 | -52.8596 | 60.48 | 0.1366 |
| | 2 | $5^1 1^1$ | 18455.8606 | -41.2479 | 85.46 | 0.1926 |
| | 3 | $1^3$ | 18462.2750 | -34.8353 | 163.1 | 0.3670 |
| | 4 | $5^1$ | 18467.4742 | -29.6361 | 54.95 | 0.1234 |
| | 5 | $1^2$ | 18473.8868 | -23.2235 | 373.8 | 0.8386 |
| | 6 | $1^1$ | 18485.4985 | -11.6118 | 513.2 | 1.149 |
| | 7 | 0 | 18497.1103 | 0 | 321.3 | 0.7171 |

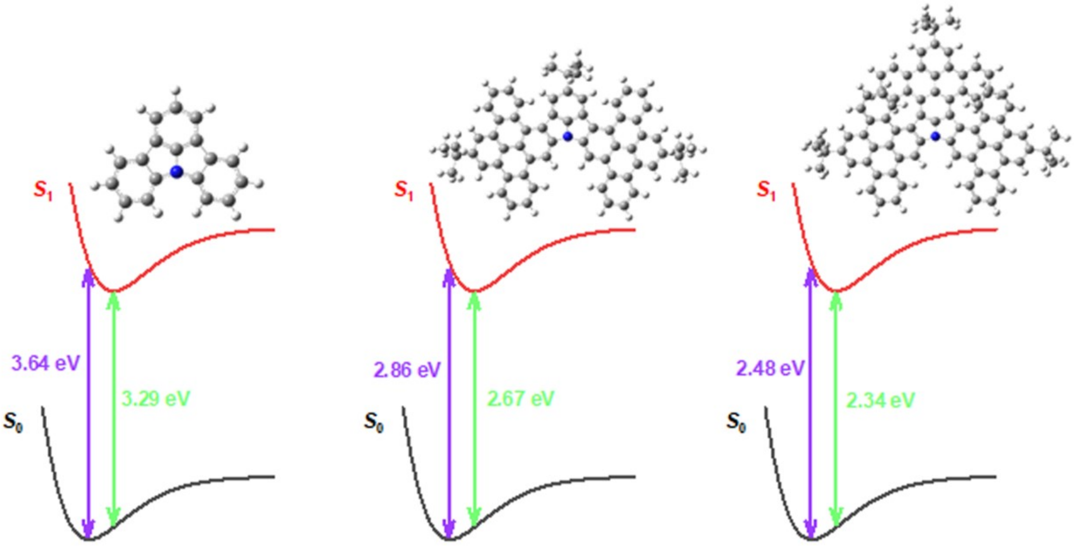
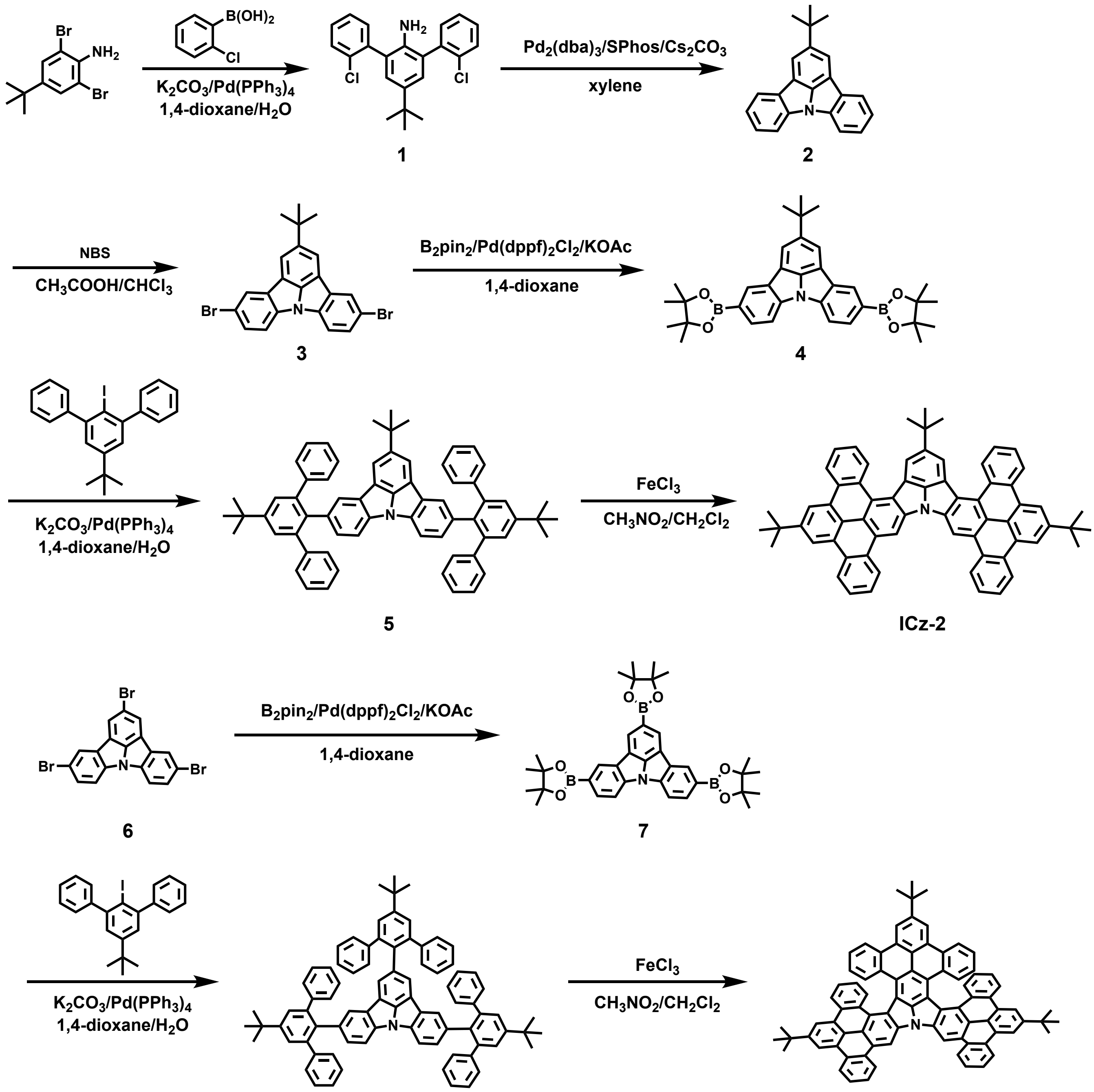



**Fig. S1** The potential energy surfaces for ground and excited states ($S_0$ and $S_1$). The energy gaps were calculated at B3LYP-D3/6-31G(d,p) level for ICz (left), ICz-2 (middle) and ICz-3 (right).

## Synthesis Procedures




**Scheme S1** Synthetic procedure of ICz-2 and ICz-3.

**Synthesis of 5'-(tert-butyl)-2'-iodo-1,1':3',1''-terphenyl**: The synthetic route was referred to the reported literature.[6]

**Synthesis of 1**: 2,6-dibromo-4-(*tert*-butyl)aniline (4.50 g, 14.66 mmol, 1.0 equiv.), (2-chlorophenyl)boronic acid (9.17 g, 58.63 mmol, 4.0 equiv.), potassium carbonate ($K_2CO_3$) (16.21 g, 117.28 mmol, 8.0 equiv.) were added with water (20 mL) and 1,4-dioxane (100 mL) into a two-neck round-bottom flask. Subsequently, tetrakis(triphenylphosphine)palladium(0) ($Pd(PPh_3)_4$) (855 mg, 0.74 mmol, 5% equiv.) was added. The mixture was degassed with nitrogen for three times, then heated to reflux and stirred overnight. After cooling to room temperature, the reaction mixture was extracted with dichloromethane and water, and the combined organic layer was condensed by rotary evaporation. The crude product was further purified by column chromatography with a mixed eluent of dichloromethane/petroleum ether (2/3) to afford viscous colorless oil (4.65 g, 86%). $^{1}$H NMR (400 MHz, DMSO-$d_6$) δ: 7.58 (ddd, $J$ = 7.5, 3.4, 1.6 Hz, 2H), 7.41 (dt, $J$ = 6.3, 2.6 Hz, 6H), 6.98 (d, $J$ = 1.2 Hz, 2H), 3.75 (d, J = 9.1 Hz, 2H), 1.25 (s, 9H). $^{13}$C NMR (75 MHz, DMSO-$d_6$) δ: 140.00, 139.87, 138.81, 138.73, 138.66, 138.63, 133.54, 133.46, 132.65, 132.62, 130.31, 130.26, 129.72, 128.07, 128.04, 127.22, 127.15, 124.57, 124.42, 34.03, 31.86. HR-MS (MALDI-TOF): calcd. for $C_{22}H_{22}Cl_2N$ [M]+ 370.1124; Found: 370.1123.

**Synthesis of 2**: Compound 1 (4.50 g, 12.15 mmol, 1.0 equiv.), SPhos (2.00 g, 4.86 mmol, 40% equiv.), cesium carbonate ($Cs_2CO_3$) (39.59 g, 121.50 mmol, 10.0 equiv.) were added with xylene (100 mL) into a two-neck round-bottom flask. Subsequently, tris(dibenzylideneacetone)dipalladium (0) ($Pd_2(dba)_3$) (1.11 g, 1.22 mmol, 10% equiv.) was added. The mixture was degassed with nitrogen for three times, then heated to reflux and stirred for 48 hours. After cooling to room temperature, the reaction mixture was extracted with dichloromethane and water, and the combined organic layer was condensed by rotary evaporation. The crude product was further purified by column chromatography with petroleum ether as eluent to afford a white powder (2.97 g, 82%). $^{1}$H NMR (300 MHz, DMSO-$d_6$) δ: 8.40 – 8.22 (m, 6H), 7.60 (t, $J$ = 7.7 Hz, 2H), 7.40 (t, $J$ = 7.6 Hz, 2H), 1.54 (s, 9H). $^{13}$C NMR (75 MHz, Chloroform-$d$) δ: 146.89, 142.73, 139.15, 130.35, 126.49, 123.02, 121.54, 117.84, 116.83, 112.21, 35.97, 32.85. HR-MS (MALDI-TOF): calcd. for $C_{22}H_{19}N$ [M]+ 297.1512; Found: 297.1512.

**Synthesis of 3**: Compound 2 (1.00 g, 3.36 mmol, 1.0 equiv.) was added with chloroform (15 mL) and glacial acetic acid (3 mL) into a two-neck round-bottom flask. The mixture was cooled to 0°C in an ice/water bath. Subsequently, N-bromosuccinimide (NBS) (1.32 g, 7.40 mmol, 2.2 equiv.) was added in several portions. After the completion of addition of NBS, the mixture was warmed to room temperature and stirred for 6 hours. The reaction mixture was poured into ethanol (100 mL), added with saturate sodium sulfite solution (100 mL). The precipitate was collected through filtration and washed with water/ethanol to obtain white powder (1.49 g, 97%). $^{1}$H NMR (300 MHz, Chloroform-$d$) δ: 8.20 (s, 2H), 8.09 (s, 2H), 7.58 (s, 4H), 1.55 (s, 9H). $^{13}$C NMR (75 MHz, Chloroform-$d$) δ: 147.70, 137.43, 131.86, 129.24, 126.09, 117.80, 116.97, 114.81, 113.20, 36.01, 32.73. HR-MS (MALDI-TOF): calcd. for $C_{22}H_{17}Br_2N$ [M]+ 452.9722; Found: 452.9722.

**Synthesis of 4**: Compound 3 (1.40 g, 3.08 mmol, 1.0 equiv.), bis(pinacolato)diboron ($B_2pin_2$)(2.35 g, 9.23 mmol, 3.0 equiv.), potassium acetate (KOAc) (3.02 g, 30.80 mmol, 10.0 equiv.) were added with 1,4-dioxane (50 mL) into a two-neck round-bottom flask. Subsequently, [1,1'-bis(diphenylphosphino)ferrocene]dichloropalladium(II) ($Pd(dppf)_2Cl_2$) (227 mg, 0.31 mmol, 10% equiv.) was added. The mixture was degassed with nitrogen for three times, then heated to 105°C and stirred overnight. After cooling to room temperature, the reaction mixture was extracted with dichloromethane and water, and the combined organic layer was condensed by rotary evaporation. The crude product was further purified by column chromatography a mixed eluent of dichloromethane/petroleum ether (1/2) to afford a greyish powder (1.44 g, 85%). $^{1}$H NMR (300 MHz, DMSO-$d_6$) δ: 8.64 (s, 2H), 8.44 (s, 2H), 8.28 (d, $J$ = 8.0 Hz, 2H), 7.89 (d, $J$ = 8.0 Hz, 2H), 1.52 (s, 9H), 1.37 (s, 24H). $^{13}$C NMR (75 MHz, Chloroform-$d$) δ: 147.45, 142.99, 140.96, 133.19, 130.16, 129.92, 117.90, 116.98, 111.90, 83.87, 35.93, 32.75, 24.99. HR-MS (MALDI-TOF): calcd. for $C_{34}H_{41}B_2NO_4$ [M]+ 549.3228; Found: 549.3212.

**Synthesis of 5**: Compound 4 (1.20 g, 2.18 mmol, 1.0 equiv.), 5'-(tert-butyl)-2'-iodo-1,1':3',1''-terphenyl (2.70 g, 6.55 mmol, 3.0 equiv.), $K_2CO_3$ (2.41 g, 17.44 mmol, 8.0 equiv.) were added with water (10 mL) and 1,4-dioxane (50 mL) into a two-neck round-bottom flask. Subsequently, $Pd(PPh_3)_4$ (126 mg, 0.11 mmol, 5% equiv.) was added. The mixture was degassed with nitrogen for three times, then heated to reflux and stirred overnight. After cooling to room temperature, the reaction mixture was extracted with dichloromethane and water, and the combined organic layer was condensed by rotary evaporation. The crude product was further purified by column chromatography with a mixed eluent of dichloromethane/petroleum ether (1/4) to afford white powder (1.52 g, 80%). $^{1}$H NMR (300 MHz, DMSO-$d_6$) δ: 7.93 (s, 2H), 7.79 (d, $J$ = 8.4 Hz, 2H), 7.66 (s, 2H), 7.43 (s, 4H), 7.22 – 6.95 (m, 22H), 1.41 (d, $J$ = 4.8 Hz, 27H). $^{13}$C NMR (101 MHz, Methylene Chloride-$d_2$) δ: 150.20, 146.73, 142.61, 141.90, 136.99, 136.44, 133.38, 130.34, 130.01, 129.22, 127.48, 126.75, 126.02, 125.97, 117.65, 116.39, 110.76, 35.70, 34.61, 32.40, 31.17. HR-MS (MALDI-TOF): calcd. for $C_{66}H_{59}N$ [M]+ 865.4642; Found: 865.4642.

**Synthesis of ICz-2**: Compound 5 (500 mg, 0.58 mmol, 1.0 equiv.) was dissolved in 50 mL extra dry dichloromethane and added into a three-neck round-bottom flask, and iron(III) chloride ($FeCl_3$) (1.87 g, 11.54 mmol, 20.0 equiv.) was suspended in 5 mL nitromethane and placed in separating funnel. The mixture was degassed with nitrogen for 5 minutes. Then $FeCl_3$ suspension was added dropwise in an ice/water bath for 15 minutes. After the completion of addition of $FeCl_3$, the ice/water bath was removed, and the mixture was warmed to room temperature and stirred for 1 hour. 5 mL methanol were added to quench the reaction. The mixture was extracted with dichloromethane and water, and the combined organic layer was condensed by rotary evaporation. The crude product was further purified by column chromatography with a mixed eluent of dichloromethane/petroleum ether (1/4) to afford a yellow solid (380 mg, 76%). $^{1}$H NMR (500 MHz, $CD_2Cl_2CD_2Cl_2$) δ: 9.88 (dd, $J$ = 7.8, 1.8 Hz, 1H), 9.66 (s, 1H), 9.14 (d, $J$ = 8.2 Hz, 2H), 9.09 – 8.98 (m, 4H), 8.94 (s, 2H), 8.93 – 8.84 (m, 5H), 7.96 (dd, $J$ = 8.2, 6.8 Hz, 2H), 7.93 – 7.78 (m, 7H), 1.73 (s, 18H), 1.65 (s, 9H). Due to the low solubility in $CD_2Cl_2CD_2Cl_2$ and other solvents, resolved $^{13}$C NMR of ICz-2 was not obtained. HR-MS (MALDI-TOF): calcd. for $C_{66}H_{51}N$ [M]+ 857.4016; Found: 857.4016. Mean error: 0.0 ppm. Anal. Calcd for $C_{66}H_{51}N$: C,92.38; H, 5.99; N, 1.63. Found: C, 92.00; H, 6.07; N, 1.55.

**Syntheses of 6**: The synthetic routes were referred to the reported literatures.[7]

**Synthesis of 7**: Compound 6 (0.99 g, 2.07 mmol, 1.0 equiv.), $B_2pin_2$ (2.61 g, 10.32 mmol, 5.0 equiv.), KOAc (3.04 g, 30.98 mmol, 10.0 equiv.) were added with 1,4-dioxane (80 mL) into a two-neck round-bottom flask. Subsequently, $Pd(dppf)_2Cl_2$ (152 mg, 0.20 mmol, 10% equiv.) was added. The mixture was degassed with nitrogen for three times, then heated to 105°C and stirred overnight. After cooling to room temperature, the reaction mixture was extracted with dichloromethane and water, and the combined organic layer was condensed by rotary evaporation. The crude product was further purified by column chromatography with a mixed eluent of dichloromethane/petroleum ether (1/1) to afford a white powder (1.06 g, 83%). $^1$H NMR (400 MHz, Chloroform-*d*) δ: 8.64 (s, 2H), 8.56 (s, 2H), 8.01 (d, *J* = 8.0 Hz, 2H), 7.92 (d, *J* = 8.1 Hz, 2H), 1.42 (d, *J* = 6.5 Hz, 36H). $^{13}$C NMR (101 MHz, Chloroform-*d*) δ: 146.29, 140.74, 133.38, 130.18, 129.86, 126.47, 118.37, 111.85, 83.84, 83.74, 25.02, 24.98. HR-MS (MALDI-TOF): calcd. for $C_{36}H_{44}B_3NO_6$ [M]+ 619.3460; Found: 619.3443.

**Synthesis of 8**: Compound 7 (1.00 g, 1.62 mmol, 1.0 equiv.), 5'-(tert-butyl)-2'-iodo-1,1':3',1''-terphenyl (2.66 g, 6.46 mmol, 4.0 equiv.), $K_2CO_3$ (2.39 g, 16.20 mmol, 10.0 equiv.) were added with water (10 mL) and 1,4-dioxane (50 mL) into a two-neck round-bottom flask. Subsequently, $Pd(PPh_3)_4$ (94 mg, 0.08 mmol, 5% equiv.) was added. The mixture was degassed with nitrogen for three times, then heated to reflux and stirred overnight. After cooling to room temperature, the reaction mixture was extracted with dichloromethane and water, and the combined organic layer was condensed by rotary evaporation. The crude product was further purified by column chromatography with a mixed eluent of dichloromethane/petroleum ether (1/3) to afford white powder (1.44 g, 81%). $^1$H NMR (400 MHz, DMSO-$d_6$) δ: 7.68 (d, *J* = 8.3 Hz, 2H), 7.45 – 7.34 (m, 8H), 7.30 (s, 2H), 7.06 (dddd, *J* = 16.7, 12.7, 8.0, 4.0 Hz, 30H), 6.93 (dd, *J* = 8.3, 1.7 Hz, 2H), 1.45 – 1.37 (m, 27H). $^{13}$C NMR (75 MHz, Methylene Chloride-$d_2$) δ: 150.14, 149.91, 142.67, 142.55, 142.45, 142.21, 141.88, 137.51, 136.58, 136.28, 134.49, 133.10, 130.21, 129.94, 128.87, 127.49, 127.36, 126.73, 126.68, 126.27, 126.02, 125.89, 122.85, 116.96, 110.55, 34.60, 31.16. HR-MS (MALDI-TOF): calcd. for $C_{84}H_{71}N$ [M]+ 1093.5581; Found: 1093.5568.

**Synthesis of ICz-3**: Compound 8 (500 mg, 0.46 mmol, 1.0 equiv.) was dissolved in 50 mL extra dry dichloromethane and added into a three-neck round-bottom flask, and $FeCl_3$ (2.23 g, 13.70 mmol, 30.0 equiv.) was suspended in 5 mL nitromethane and placed in separating funnel. The mixture was degassed with nitrogen for 5 minutes. The $FeCl_3$ suspension was added dropwise in an ice/water bath for 15 minutes. After the completion of addition of $FeCl_3$, the ice/water bath was removed, and the mixture was warmed to room temperature and stirred for 1 hour. 5 mL methanol were added to quench the reaction. The mixture was extracted with dichloromethane and water, and the combined organic layer was condensed by rotary evaporation. The crude product was further purified by column chromatography with a mixed eluent of dichloromethane/petroleum ether (1/4) to afford an orange solid (340 mg, 68%). ICz-3 should be comprised of diastereomers as it structurally features [6]helicene segments. We herein do not discuss the behaviour of each diastereomer as we investigate the collective photophysical behaviour. $^1$H NMR (500 MHz, $CD_2Cl_2CD_2Cl_2$) δ: 9.94 (s, 1H), 9.29 – 9.17 (m, 4H), 9.17 – 9.05 (m, 5H), 8.94 (d, *J* = 8.2 Hz, 3H), 8.85 (d, *J* = 8.1 Hz, 2H), 8.77 (d, *J* = 8.2 Hz, 2H), 8.36 (d, *J* = 8.0 Hz, 1H), 8.05 – 7.80 (m, 6H), 7.48 (dt, *J* = 20.5, 7.4 Hz, 4H), 6.60 (t, *J* = 7.5 Hz, 2H), 6.52 (t, *J* = 7.4 Hz, 2H), 1.87 (s, 9H), 1.84 (s, 18H). Due to the low solubility in $CD_2Cl_2CD_2Cl_2$ and common solvents, $^{13}$C NMR of ICz-3 was not recorded. HR-MS (MALDI-TOF): calcd. for $C_{84}H_{59}N$ [M]+ 1081.4642; Found: 1081.4639. Mean error: -0.2 ppm. Anal. Calcd for $C_{84}H_{59}N$: C,93.21; H, 5.49; N, 1.29. Found: C, 93.03; H, 5.29; N, 1.17.

**Synthesis of dibenzo[*e,l*]pyrene (DBP)**: The synthetic route was referred to the reported literature.[8,9]

## Mass Spectra

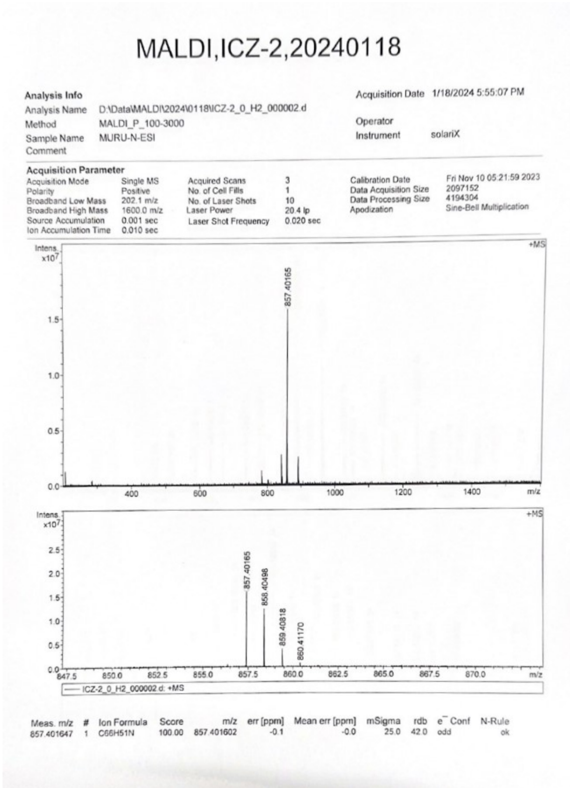


**Fig. S2** The HR-MALDI-TOF mass spectra of ICz-2

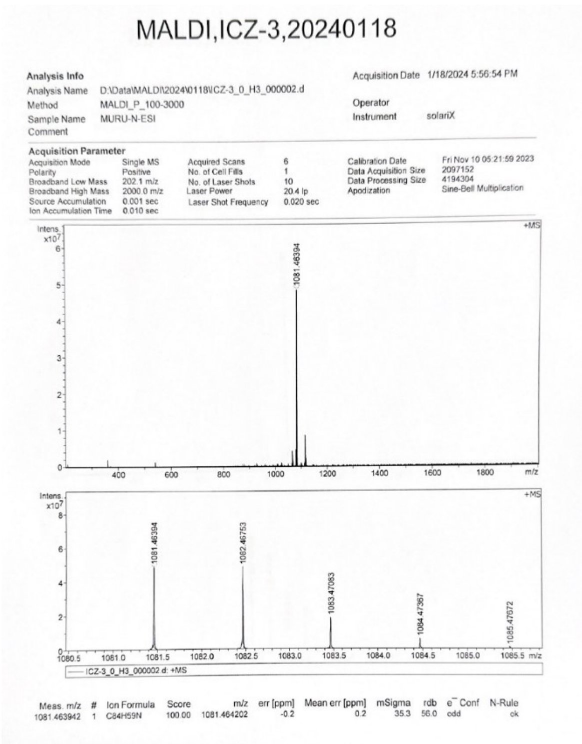


**Fig. S3** The HR-MALDI-TOF mass spectra of ICz-3.

## NMR of New Compounds

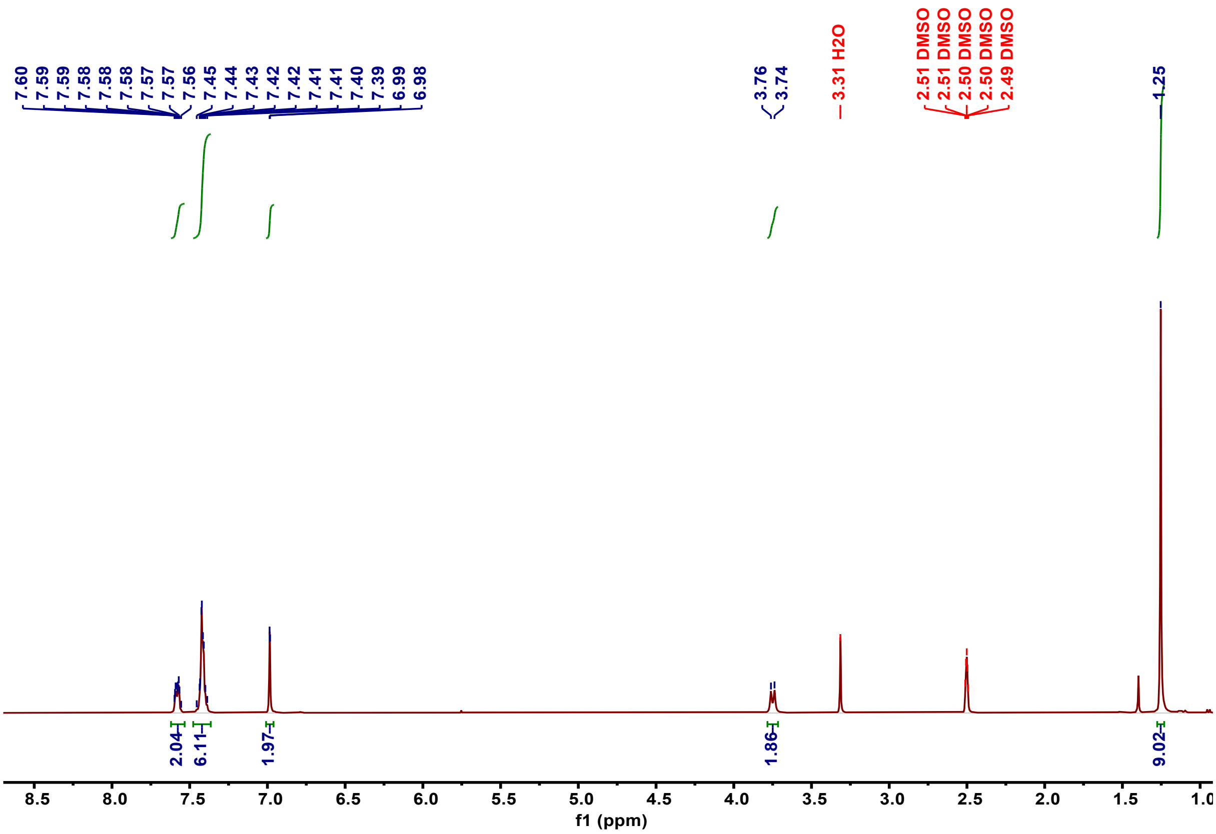



**Fig S4** $^1$H NMR spectrum of compound **1** (400MHz, DMSO-$d_6$).

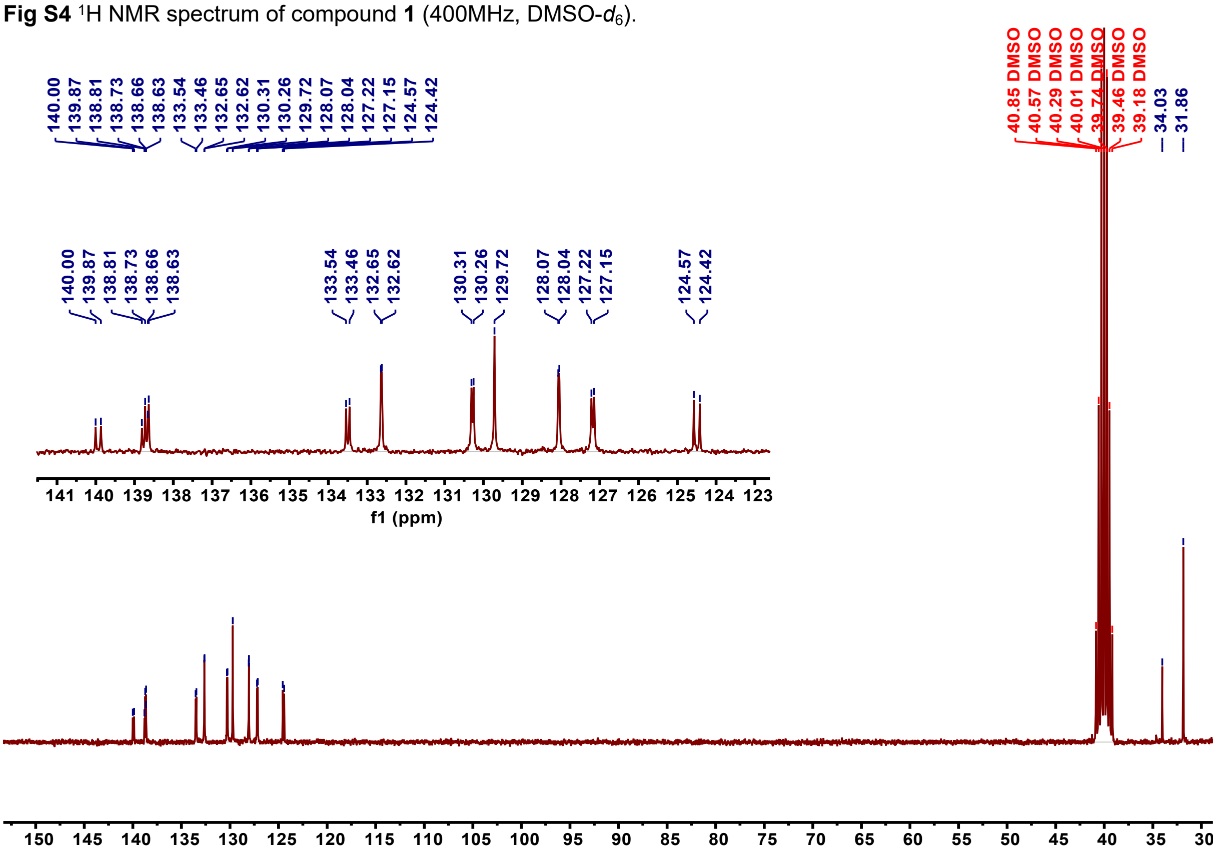


**Fig. S5** $^{13}$C NMR spectrum of compound **1** (75MHz, DMSO-$d_6$).

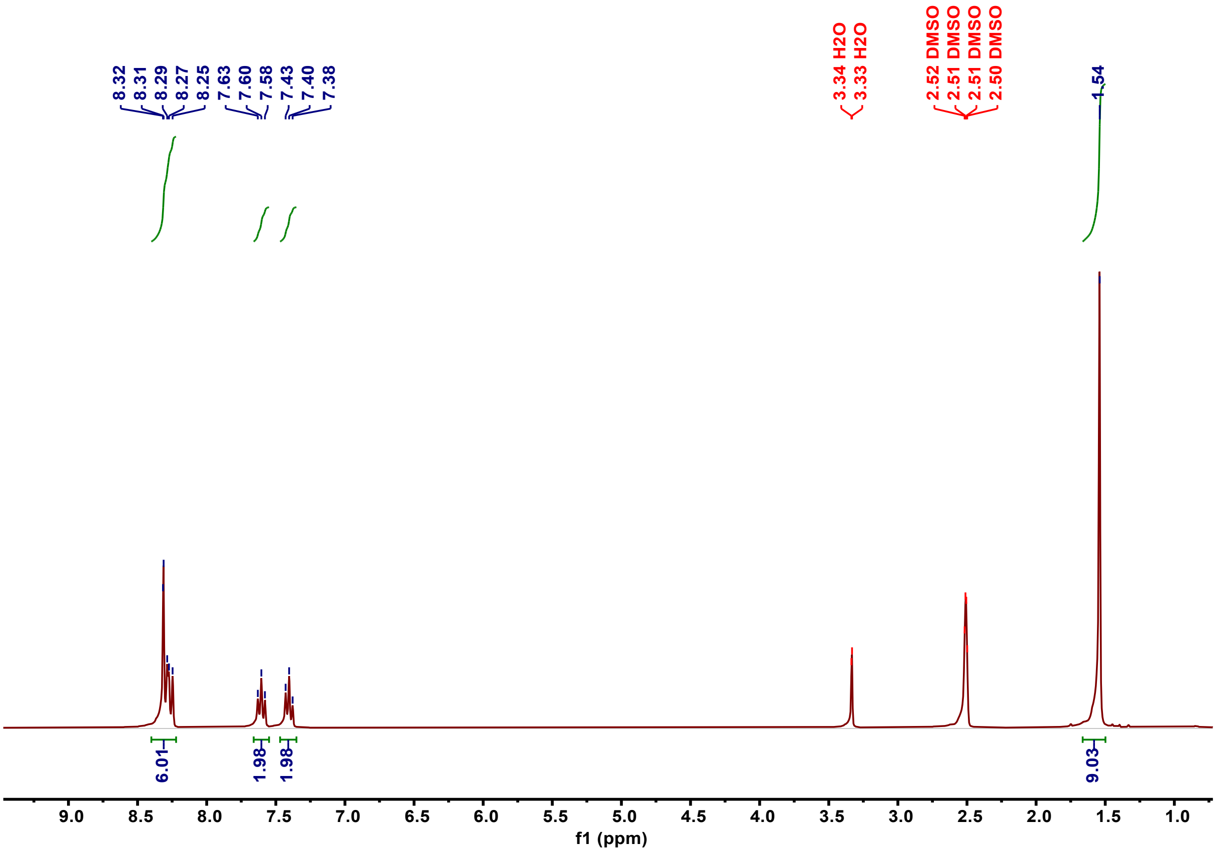



**Fig. S6** $^{1}$H NMR spectrum of compound **2** (300MHz, DMSO-$d_6$).

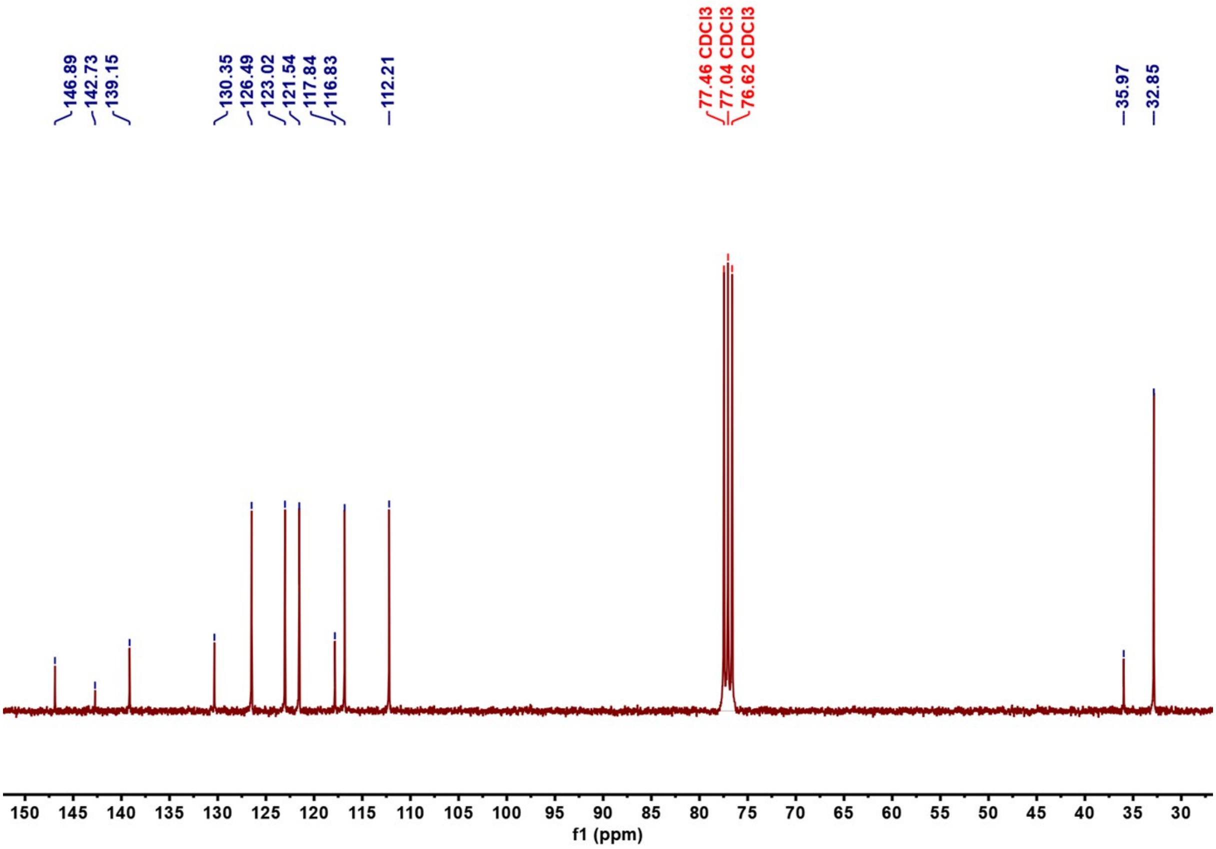



**Fig. S7** $^{13}$C NMR spectrum of compound **2** (75MHz, DMSO-$d_6$).

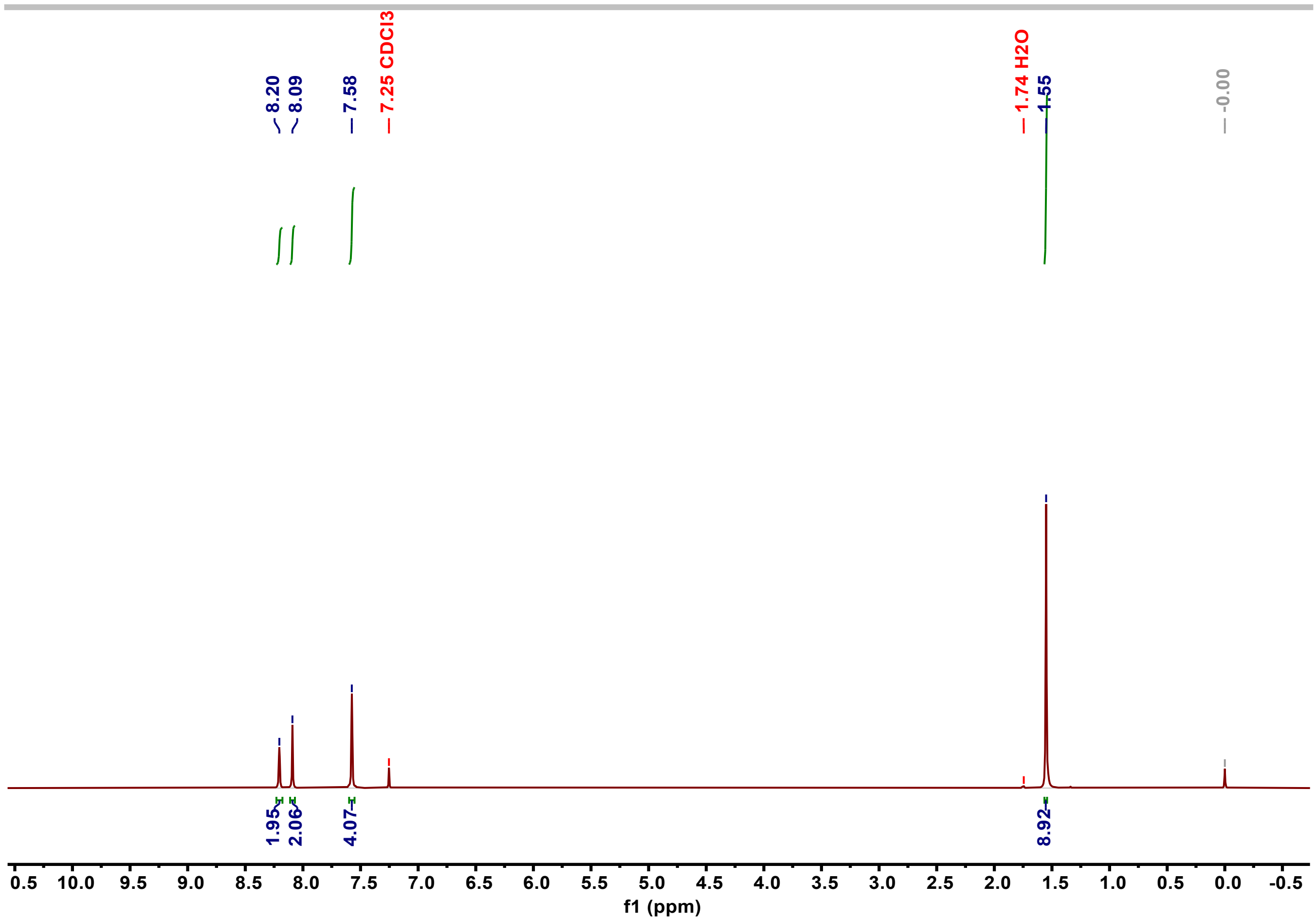



**Fig. S8** [1]H NMR spectrum of compound **3** (300MHz, Chloroform-*d*).

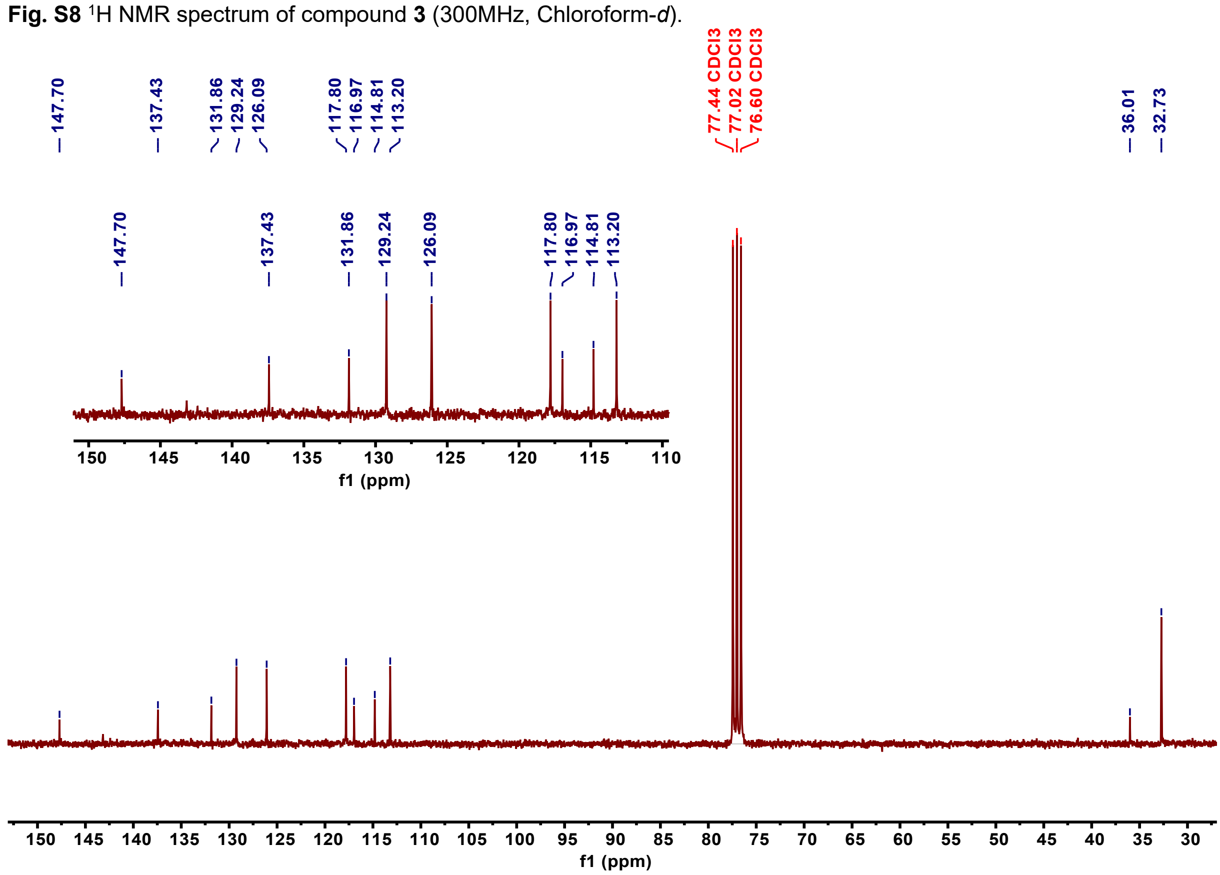



**Fig. S9** [13]C NMR spectrum of compound **3** (75MHz, Chloroform-*d*).

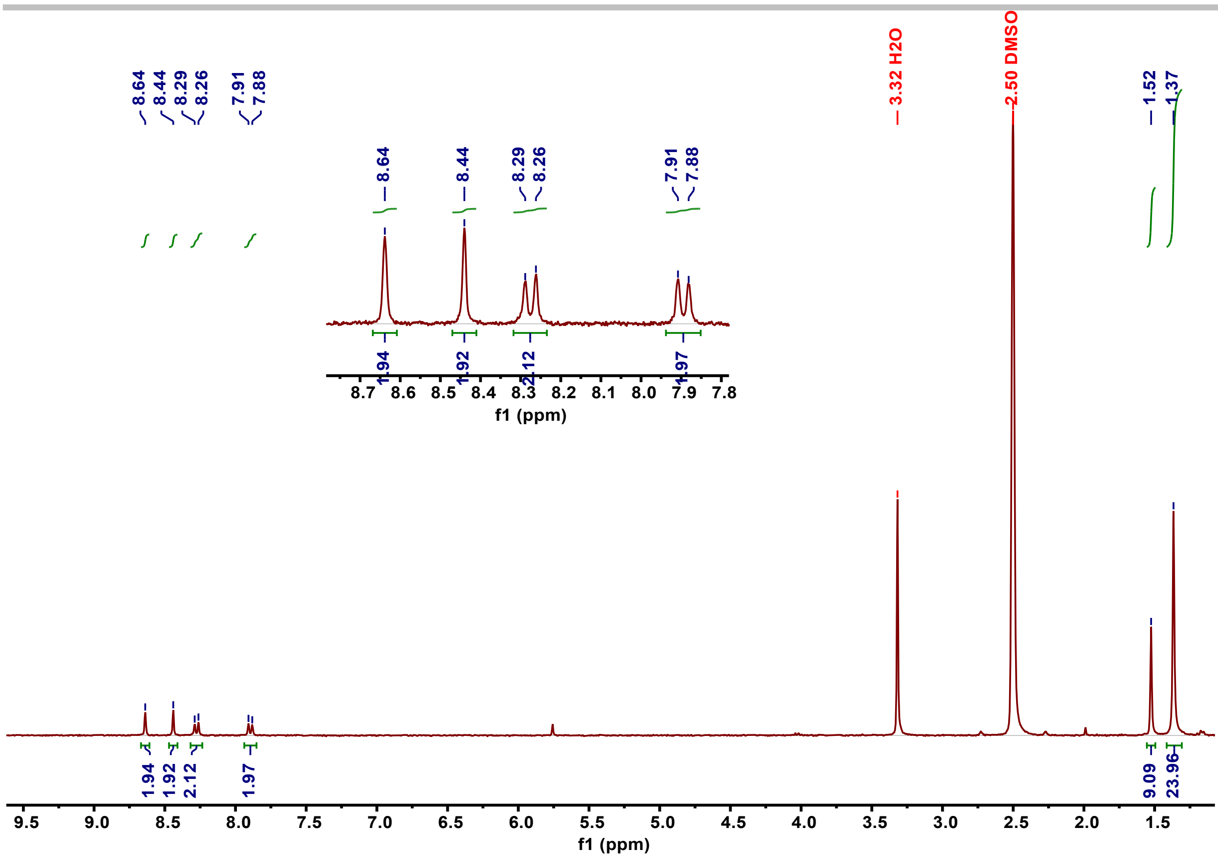


**Fig. S10** [1]H NMR spectrum of compound **4** (300MHz, DMSO-$d_6$).

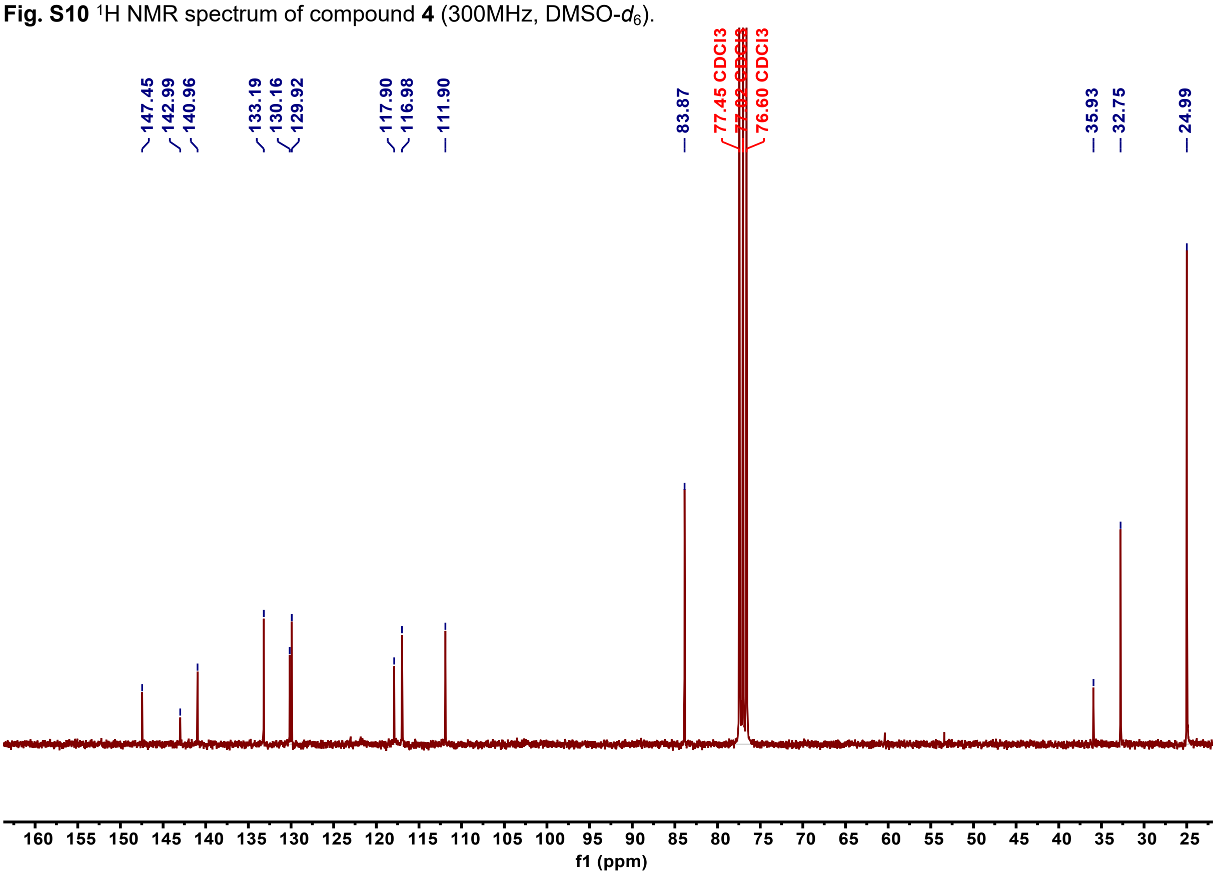


**Fig. S11** [13]C NMR spectrum of compound **4** (75MHz, Chloroform-*d*).

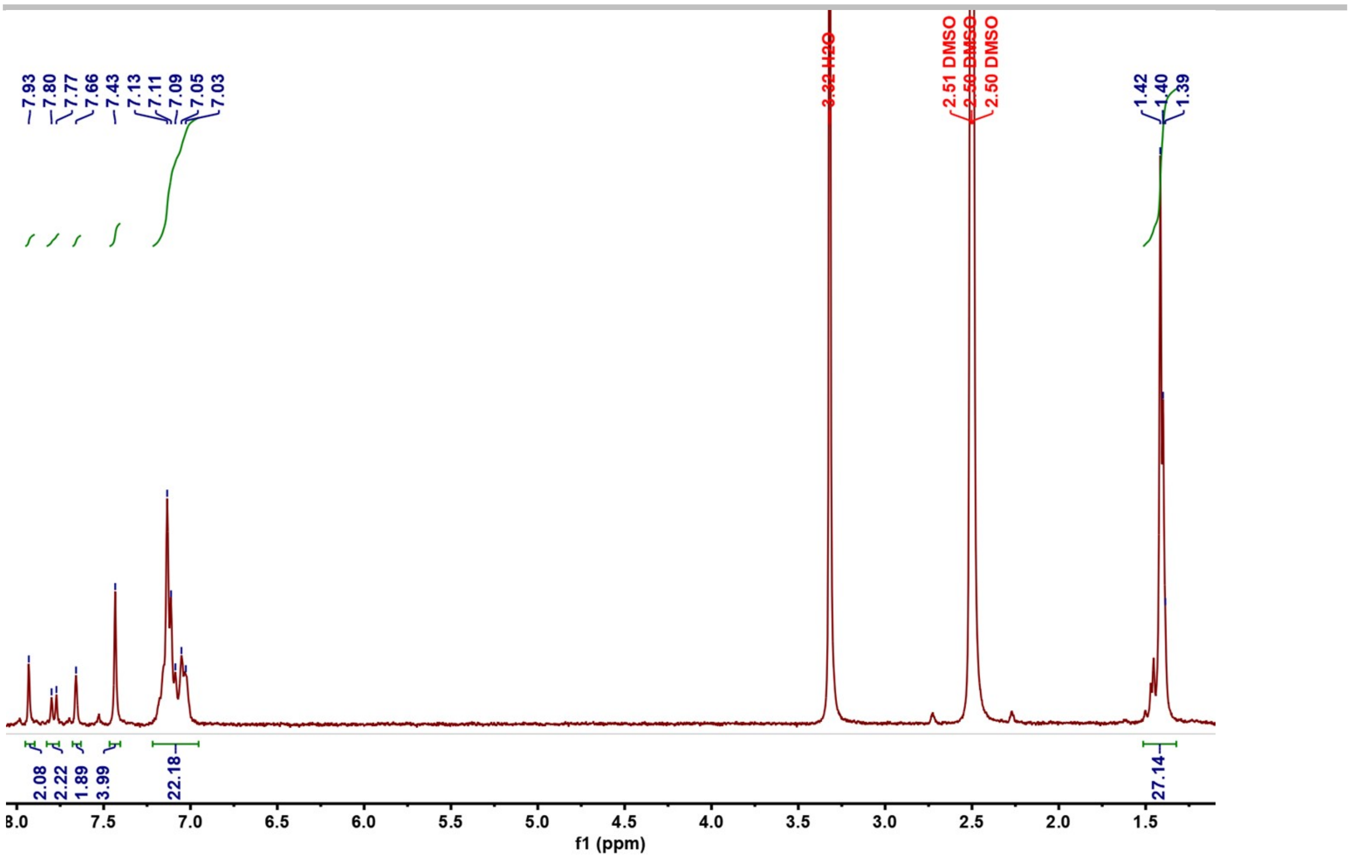



**Fig. S12** [1]H NMR spectrum of compound **5** (300MHz, DMSO-$d_6$).

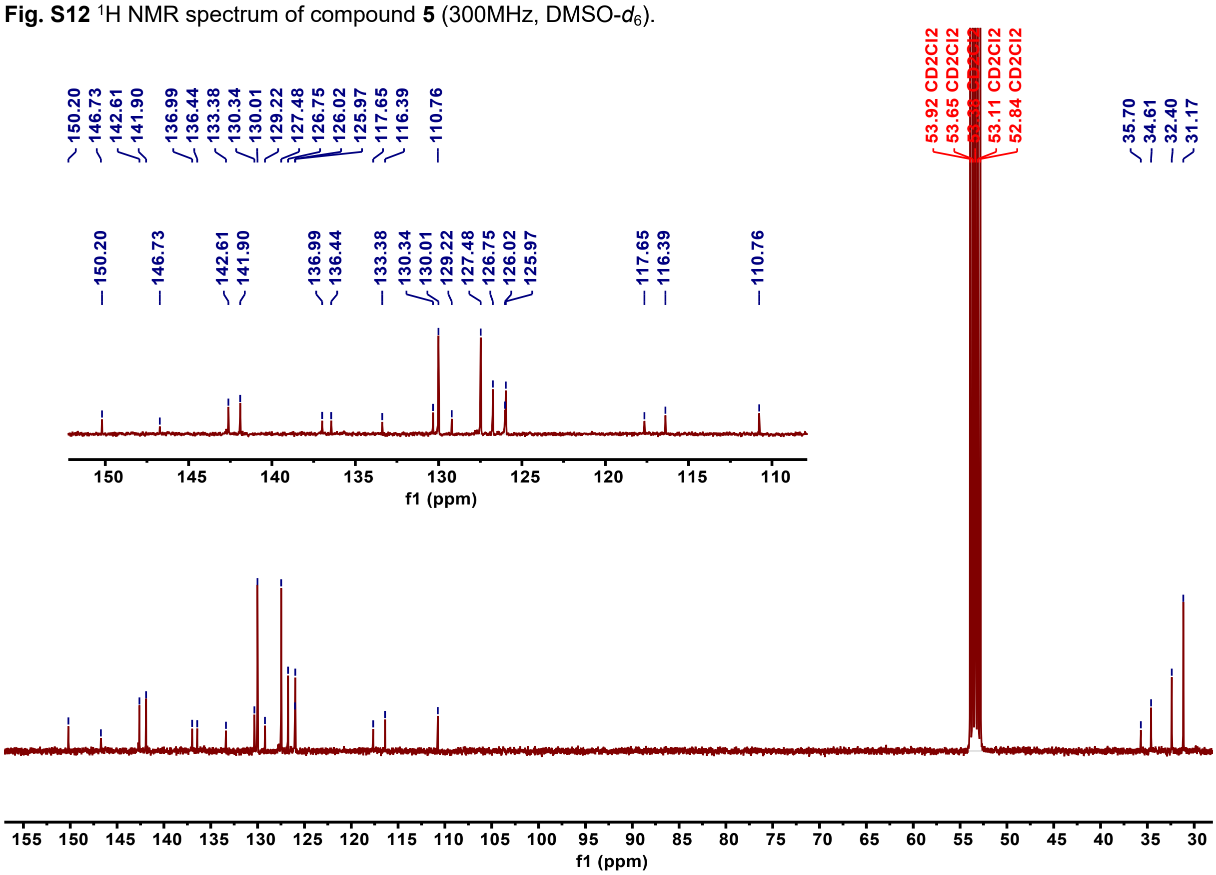



**Fig. S13** [13]C NMR spectrum of compound **5** (101 MHz, Methylene Chloride-$d_2$).

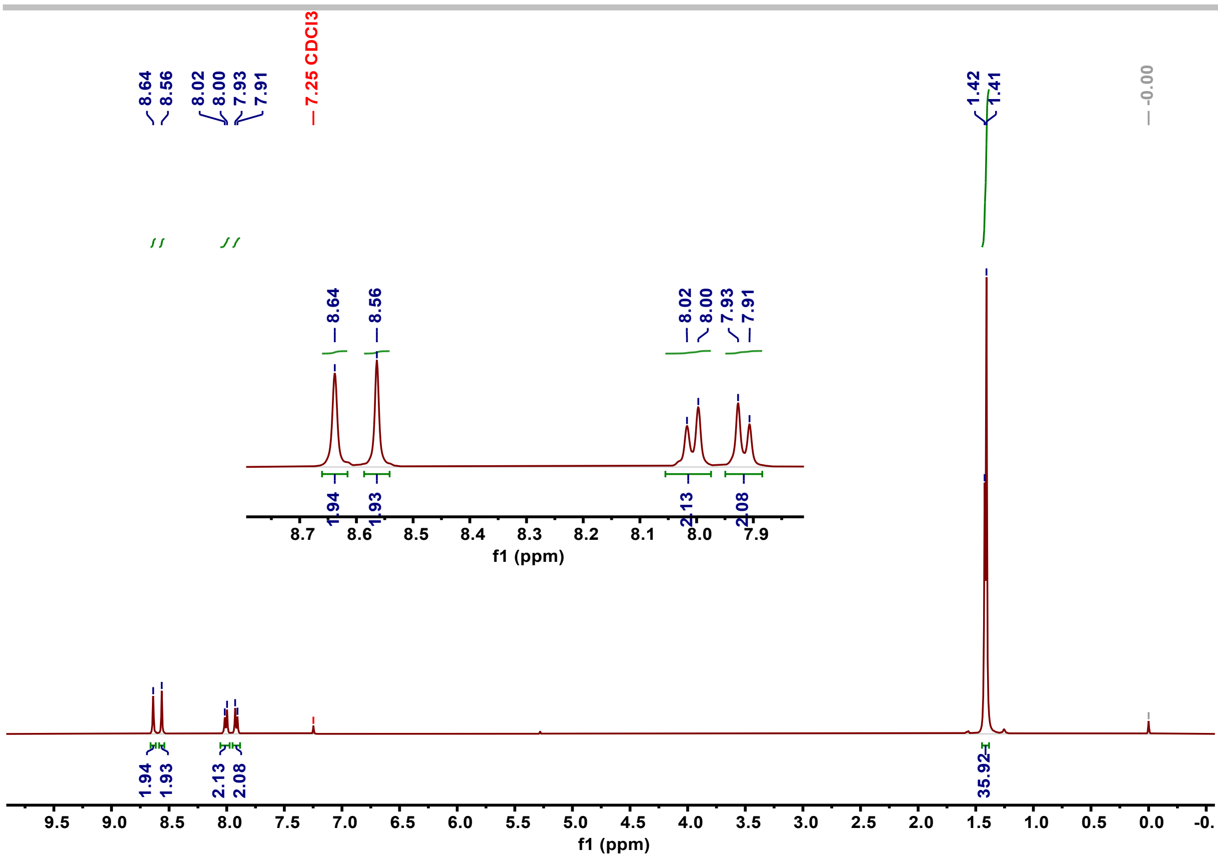



**Fig. S14** [1]H NMR spectrum of compound **7** (400MHz, Chloroform-*d*).

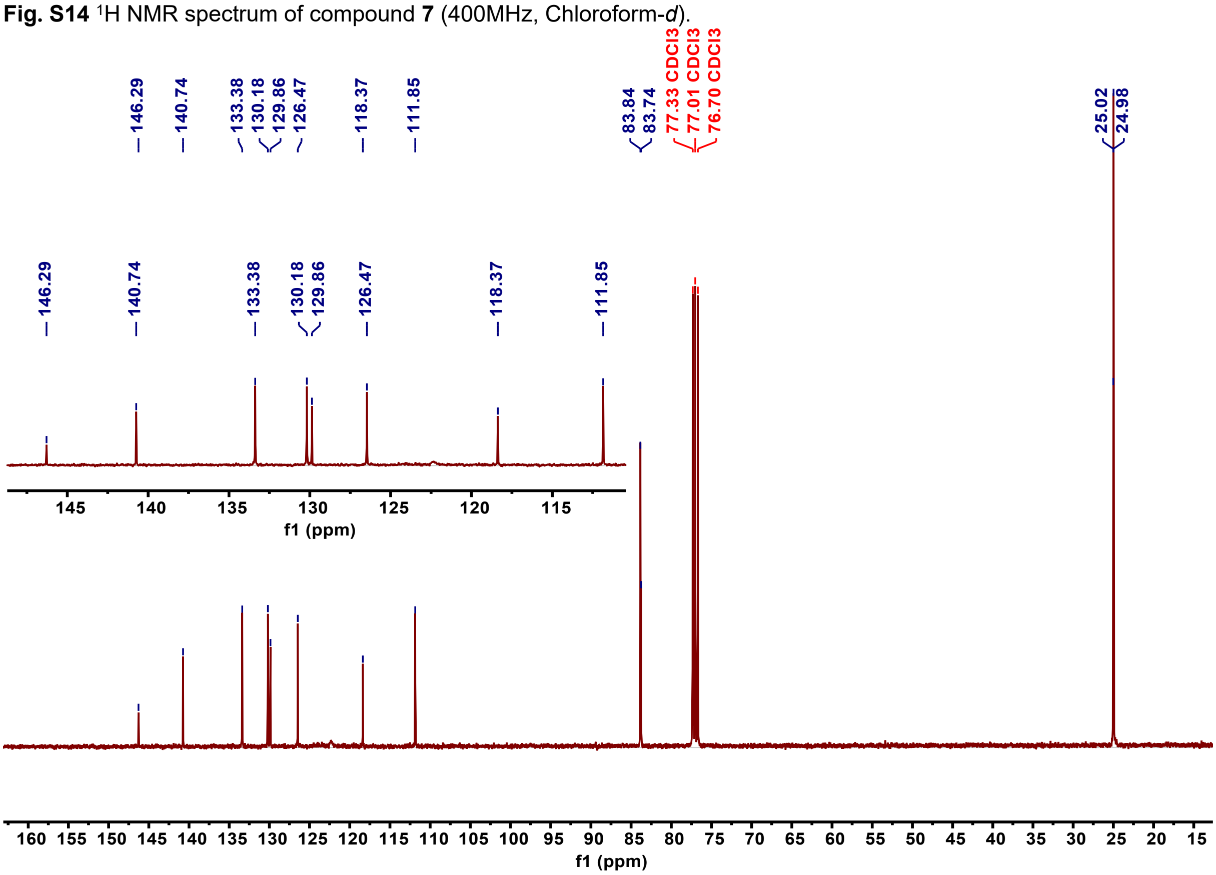



**Fig. S15** [13]C NMR spectrum of compound **7** (101MHz, Chloroform-*d*).

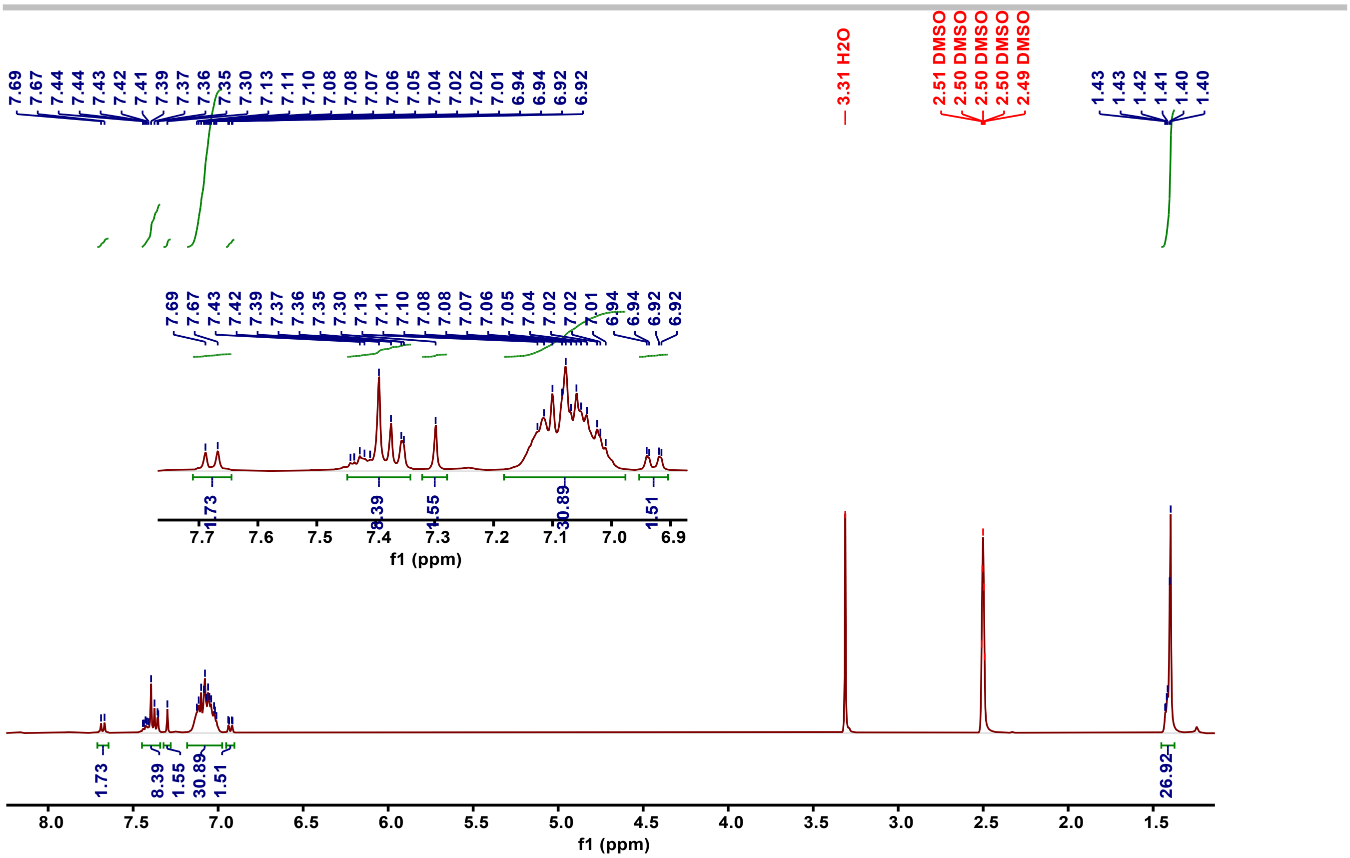


**Fig. S16** [1]H NMR spectrum of compound **8** (400MHz, DMSO-$d_6$).

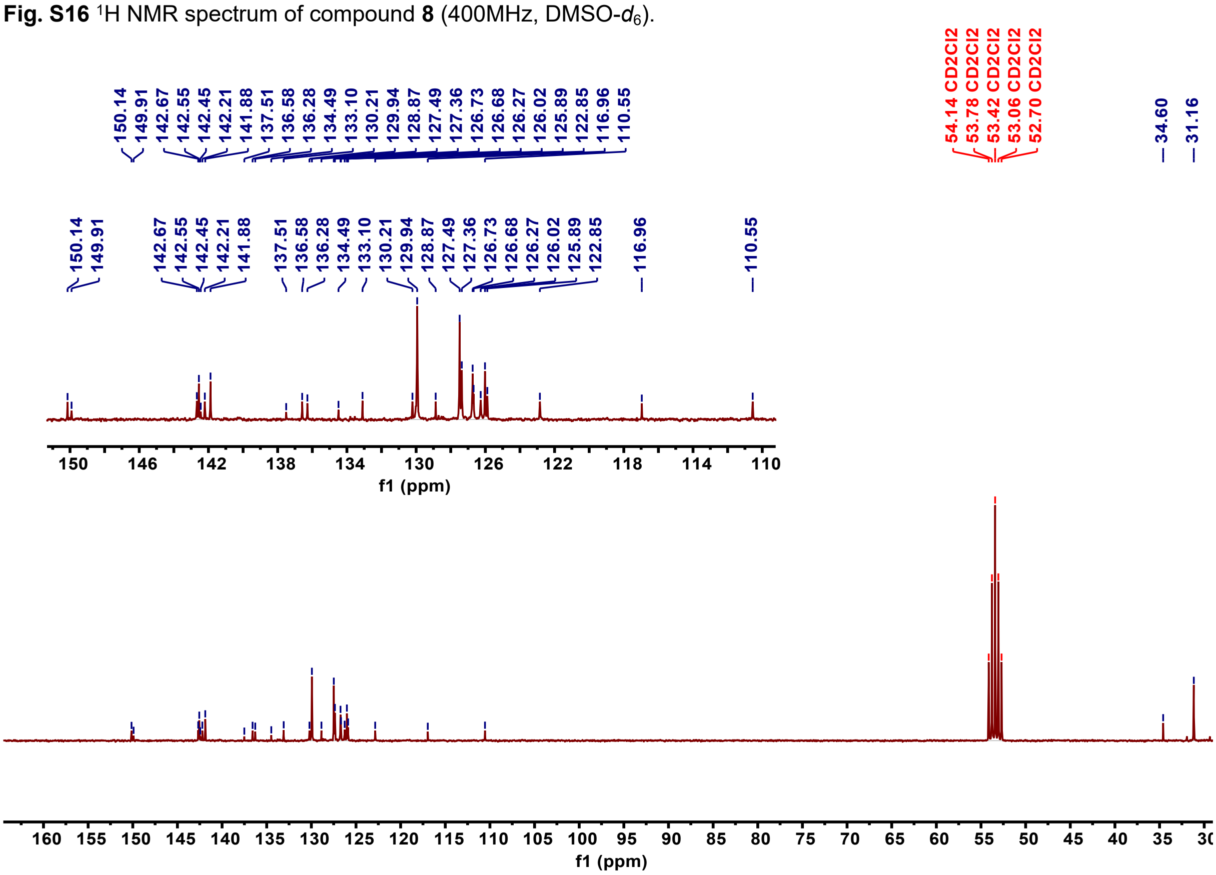


**Fig. S17** [13]C NMR spectrum of compound **8** (75MHz, Methylene Chloride-$d_2$).

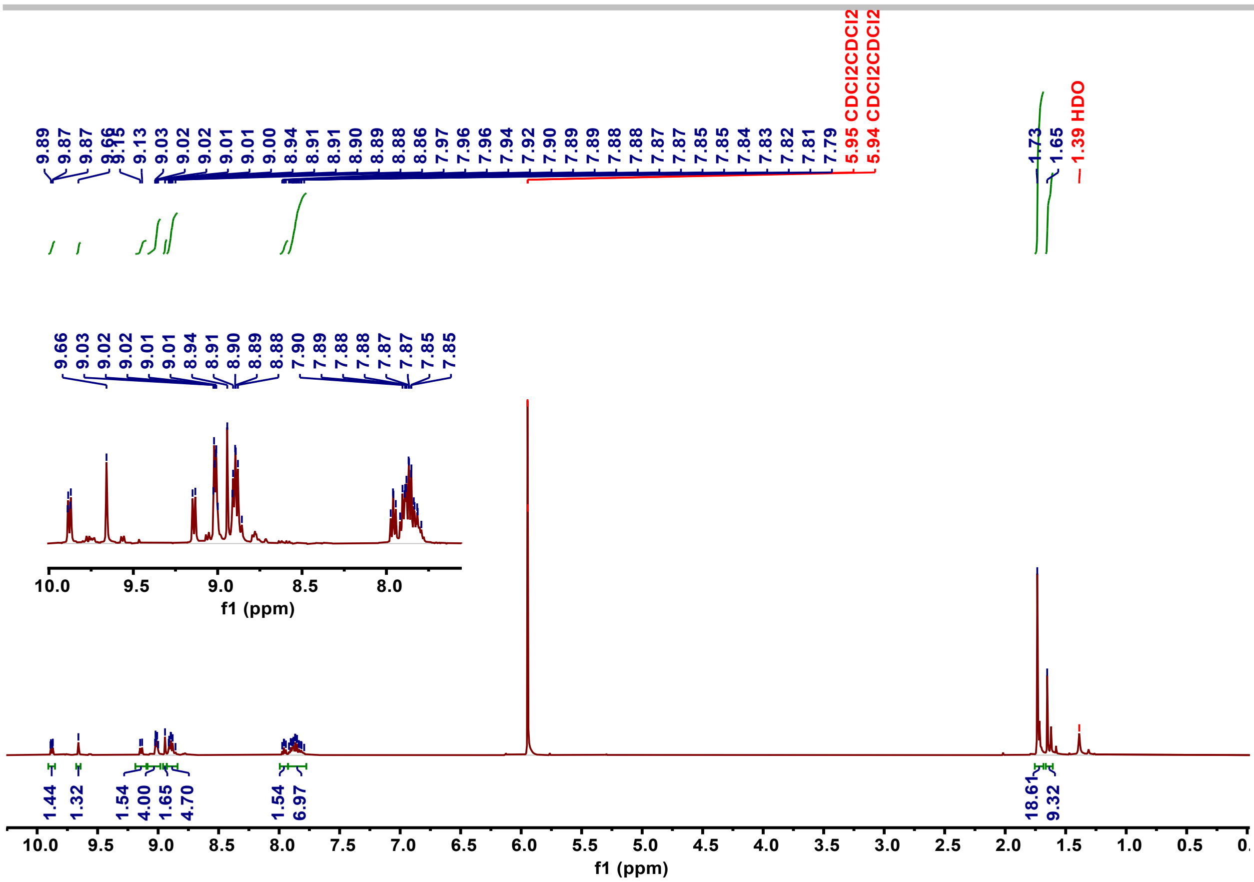



**Fig. S18** $^1$H NMR spectrum of **ICz-2** (500MHz, $CD_2Cl_2CD_2Cl_2$, measured in 493 K).

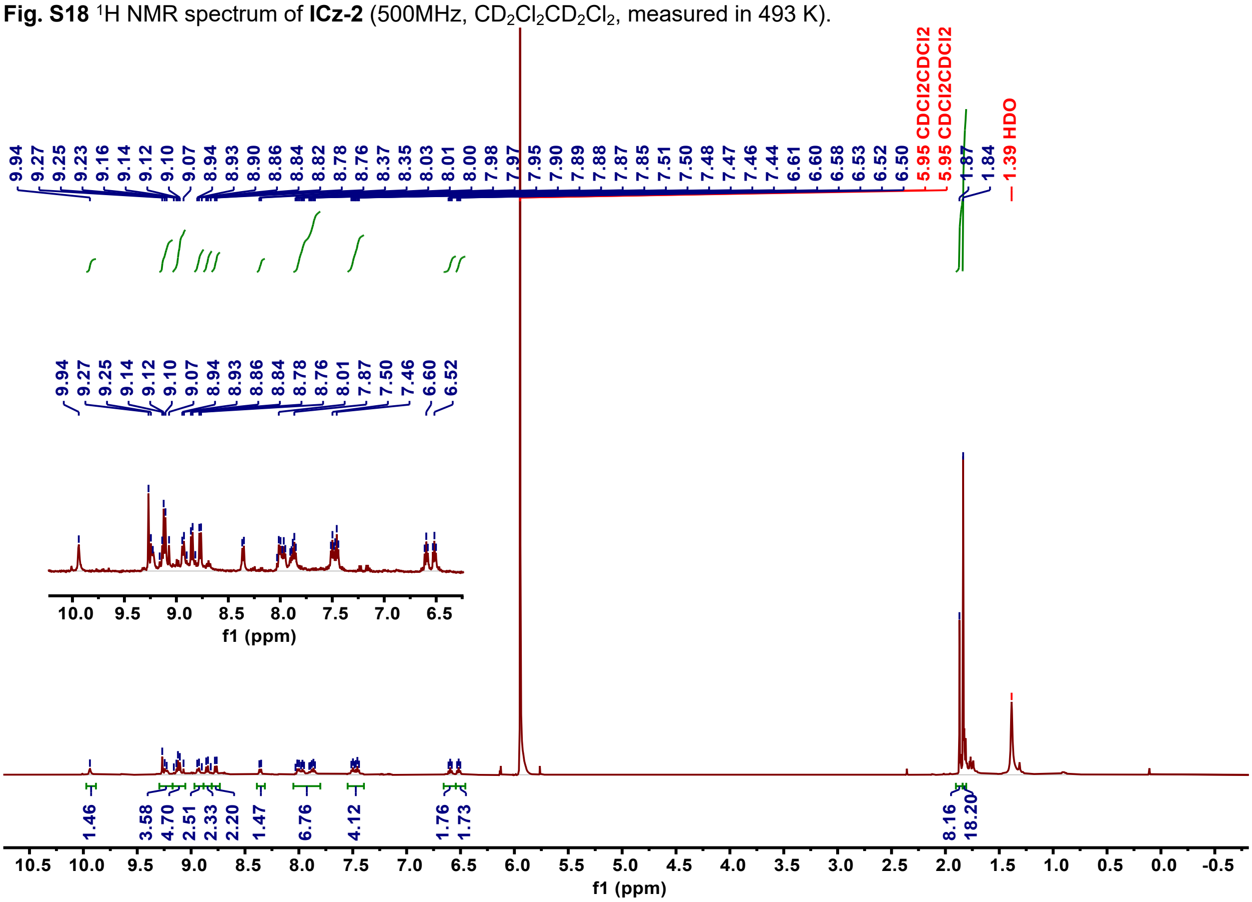



**Fig. S19** $^1$H NMR spectrum of **ICz-3** (500MHz, $CD_2Cl_2CD_2Cl_2$, measured in 493 K).

## X-ray Crystallography

Single crystal of ICz-2 was obtained by slow evaporation of toluene/methanol solutions under ambient conditions.
The crystal data are as follows:

Complete Data:

| | Crystal Data for ICz-2 |
|---|---|
| Cell | a = 17.0229(6) Å; b = 18.2490(7) Å; c = 18.5767(7) Å;<br>α = 63.138(4)°, β = 70.133(3)°, γ = 77.364(3)° |
| Temperature | 170 K |
| Volume | 4827.1(4) |
| Space Group | P -1 |
| Hall Group | -P 1 |
| Moiety Formula | 2($C_{66}H_{51}N$) 1($C_7H_8$) |
| Sum Formula | $C_{139}H_{110}N_2$ |
| $M_r$ | 1808.28 |
| Z | 2 |
| $D_x$ | 1.244 g/cm$^3$ |
| $M_u$ | 0.535 mm$^{-1}$ |
| F000 | 1916.0 |
| h, k, $l_{max}$ | 20, 21, 22 |
| $N_{ref}$ | 16953 |
| $T_{min}$, $T_{max}$ | 0.754, 1.000 |
| Data Completeness | 0.994 |
| $\theta_{max}$ | 66.600 |
| R (reflections) | 0.0749 (12258) |
| wR2 (reflections) | 0.2189 (16953) |
| S | 1.072 |
| $N_{par}$ | 1361 |

## Thermogravimetric and Electrochemical Analysis

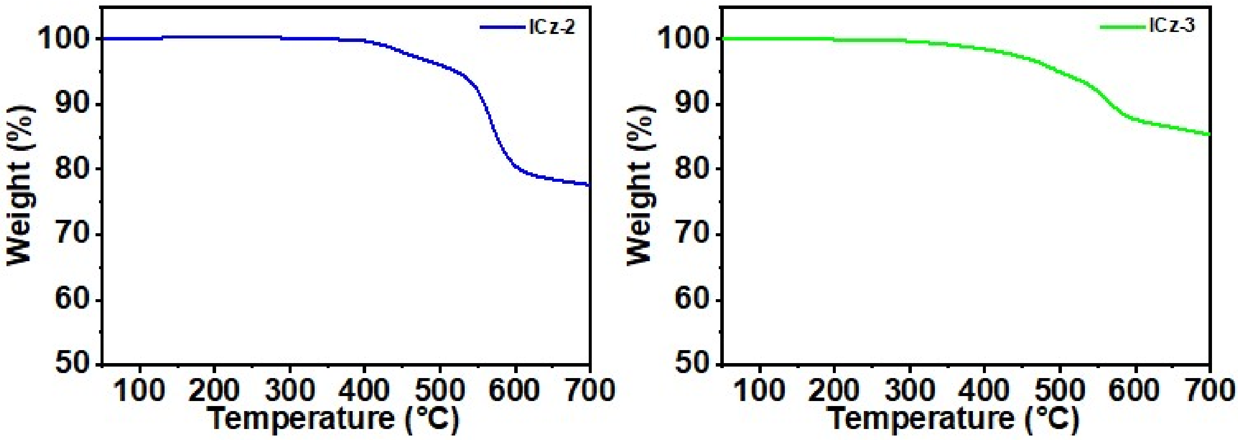



**Fig. S20** The TGA curves of ICz-2 and ICz-3.

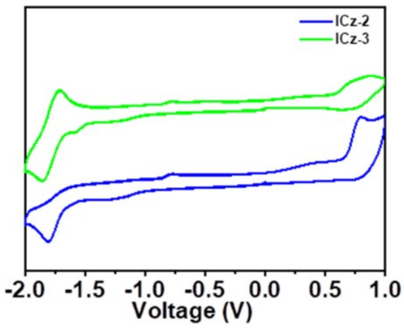



**Fig. S21** The CV curves of ICz-2 and ICz-3. The LUMO energy levels can be calculated by the reduction curves, with 3.00 eV for ICz-2 and 3.21 eV for ICz-3. Combined with the energy gap determined by the onset of absorption spectra, being 2.71 eV for ICz-2 and 2.36 eV for ICz-3, the HOMO energy levels can be obtained as 5.71 eV and 5.51 eV, respectively.

## Photophysical Properties

**Table S3** The fluorescence properties of some all-carbon and N-doped NGs

| Compound | $\lambda_{em}$ [nm] | Solvent | $\Phi_{PL}$ (%) | EQE (%) | Reference |
|---|---|---|---|---|---|
| COR | 417 | DCM | 7 | - | [10] |
| Q[6]H | 527 | DCM | 3 | - | [11] |
| HBC | 487 | DCM | 3 | - | [12] |
| Azacornnulene | 490 | DCM | 24 | - | [13] |
| DBOV | 594 | THF | 80 | - | [14] |
| DBOV-C12 | 617 | Toluene | 79 | - | [15] |
| FM-C4 | 539 | DCM | 12.9 | - | [16] |
| NS-Octulene-2 | 464, 495 | Toluene | - | - | [17] |
| Diazapentabenzocorannulenium | 491 (Water)/511 (DCM) | Water/DCM | 12 (Water)/6 (DCM) | - | [18] |
| Pyrrole-fused Thiepine | 459, 485 | DCM | 29 | - | [19] |
| **ICz-2** | **454** | **Toluene** | **92** | **3.8** | **This Work** |
| **ICz-3** | **516** | **Toluene** | **93** | **12.3** | **This Work** |

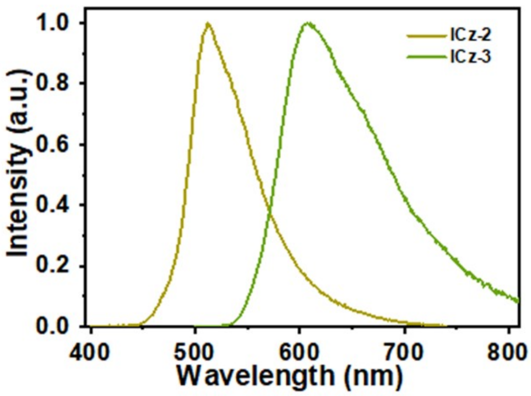



**Fig. S22** The emission spectra of a) ICz-2 and b) ICz-3 measured in grinded powder at 298 K.

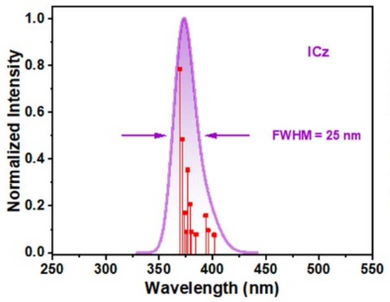



**Fig. S23** Emission spectra of ICz simulated by Franck-Condon analysis (B3LYP-D3/6-31G(d,p)) on the $S_1$-$S_0$ transition in toluene broadening with a half width at half-maximum of 300 $cm^{-1}$. Dipole strength of each transition is marked by red dots.

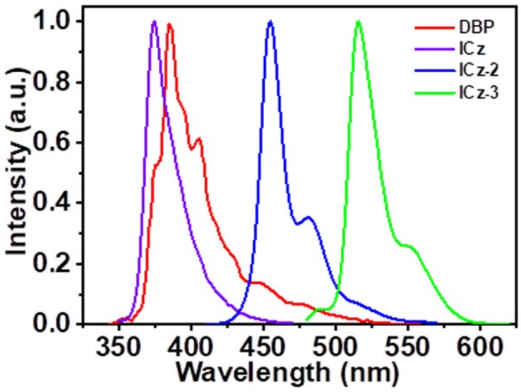



**Fig. S24** The emission spectra of ICz-2 and ICz-3 compared with ICz and DBP measure in $10^{-5}$ M toluene solution at 298 K.

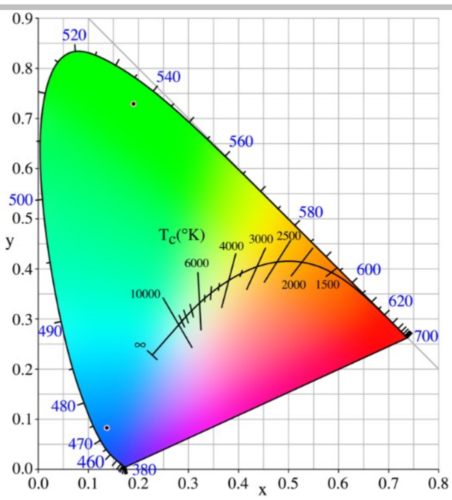



**Fig. S25** CIE graph of ICz-2 and ICz-3 based on emission spectra in toluene solutions.

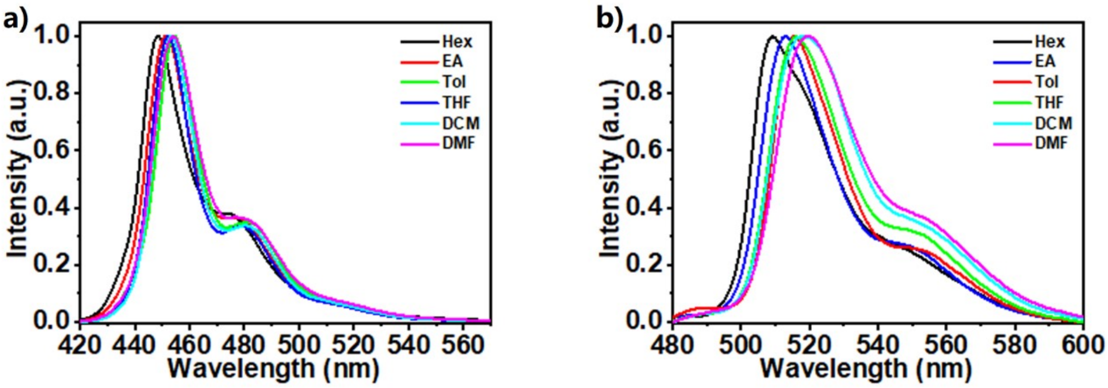



**Fig. S26** The emission spectra of a) ICz-2 and b) ICz-3 measured in multiple solvents with different polarity, including n-hexane (Hex), ethyl acetate (EA), toluene (Tol), tetrahydrofuran (THF), dichloromethane (DCM) and *N*,*N*-dimethylformamide (DMF).

**Table S4** Summary of emission spectra data in different polar solvents of ICz-2 and ICz-3

| Compound | ICz-2 | | ICz-3 | |
|---|---|---|---|---|
| Solvent | $\lambda_{em}{}^{a}$ [nm] | FWHM [nm] | $\lambda_{em}{}^{a}$ [nm] | FWHM [nm] |
| Hex | 448 | 20 | 509 | 26 |
| EA | 453 | 20 | 513 | 23 |
| Tol | 454 | 18 | 516 | 23 |
| THF | 452 | 18 | 516 | 25 |
| DCM | 453 | 18 | 518 | 29 |
| DMF | 454 | 21 | 520 | 29 |

[a] Peak wavelength of emission spectra measured in $10^{-5}$ M solutions at 298 K.

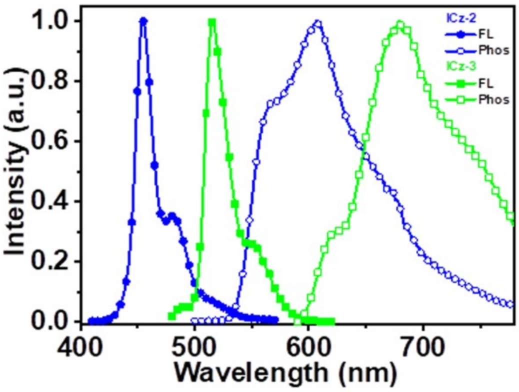



**Fig. S27** The phosphorescent emission spectrum of ICz-2 and ICz-3 in toluene solutions at 77 K, in comparison with their corresponding fluorescent emission spectrum in toluene at room temperature.

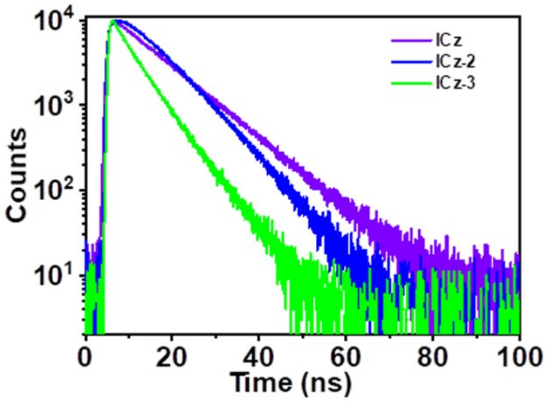



**Fig. S28** The PL decay curves of ICz, ICz-2 and ICz-3.

**Table S5** Summary of emission spectra data of ICz and DBP

| Compound | $\lambda_{em}{}^{a}$ [nm] | FWHM [nm] | $\Phi_{PL}{}^{b}$ [%] |
|---|---|---|---|
| ICz | 384 | 23 | 46 |
| DBP | 375 | 35 | 5 |

[a] Peak wavelength of PL maxima measure in $10^{-5}$ M toluene solution at 298 K. [b] Measured as absolute quantum yield in diluted toluene solution with an integrating sphere system at 298 K.

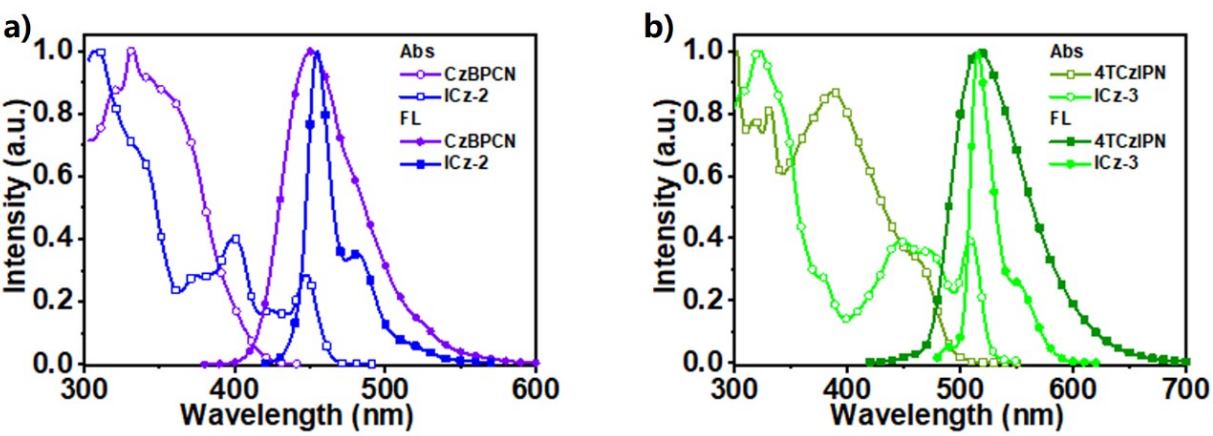



**Fig. S29** a) The absorption and emission spectra of CzBPCN and ICz-2 in toluene solutions with concentrations of $10^{-5}$ M. b) The absorption and emission spectra of 4TCzIPN and ICz-3 in toluene solutions with concentrations of $10^{-5}$ M.

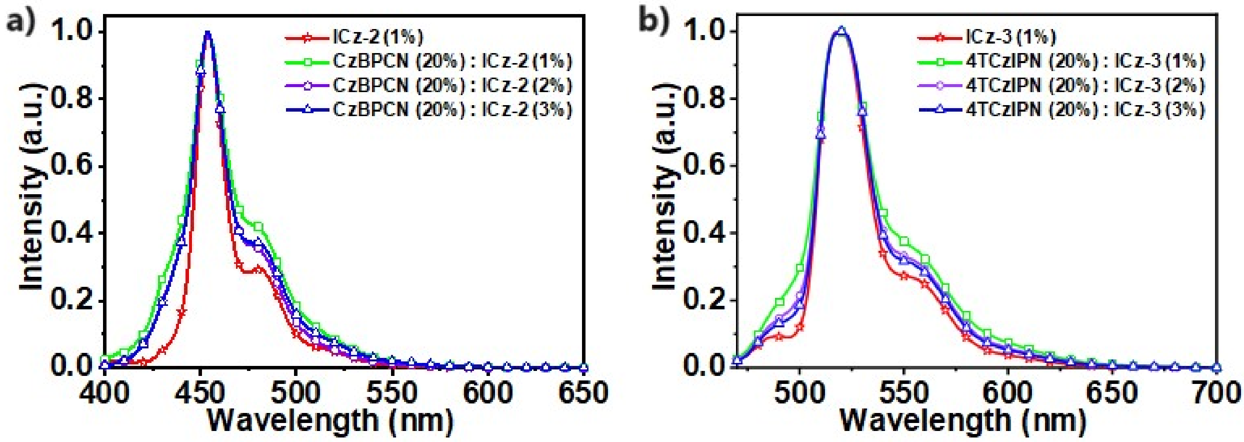



**Fig. S30** The emission spectra of ternary TSF films of a) PPF: CzBPCN: ICz-2 and b) mCBCP: 4TCzIPN: ICz-3. The concentrations in blankets are meant for weight fractions.

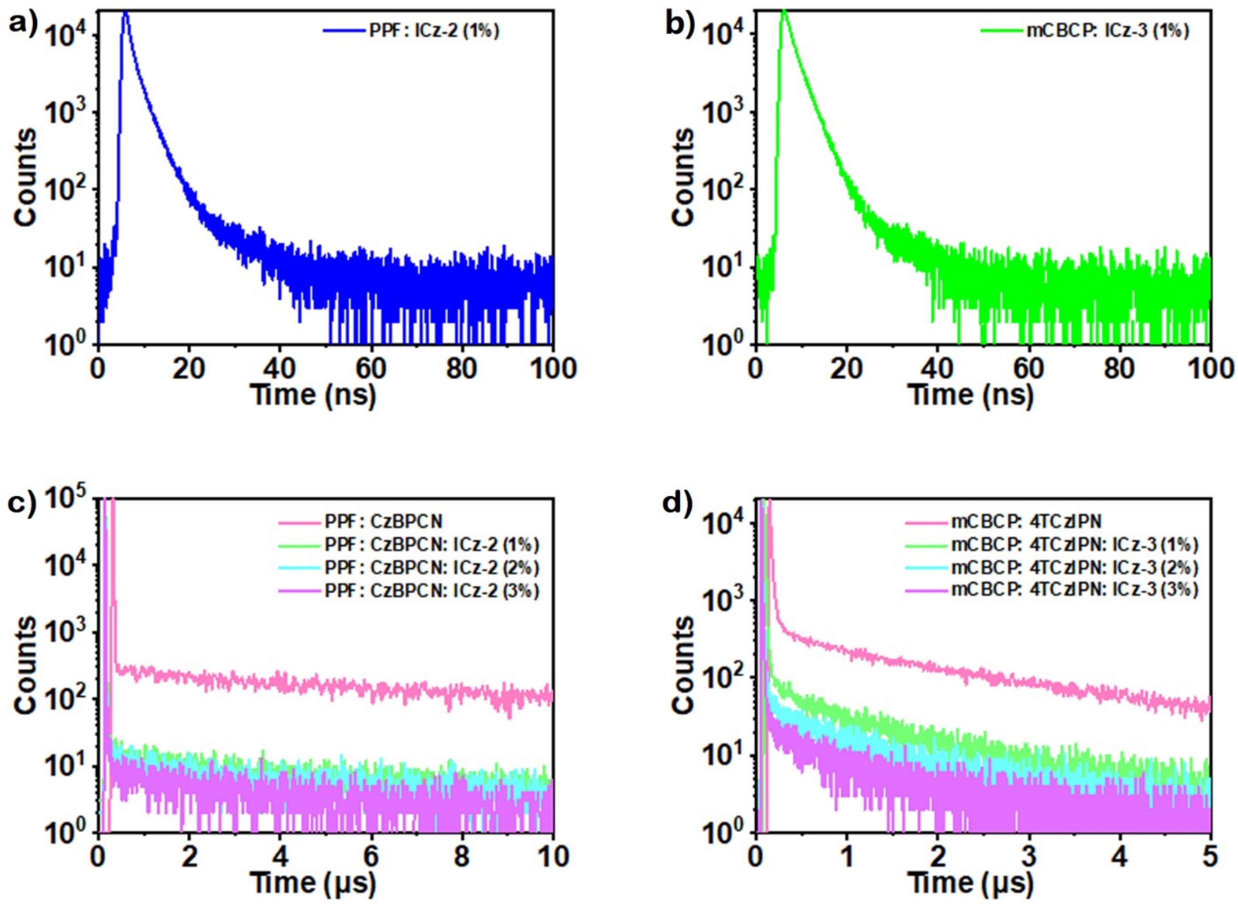



**Fig. S31** The PL decay curves of binary and ternary TSF films. The concentrations in blankets are meant for weight fractions. CzBPCN and 4TCzIPN as sensitizers are added in the portion of 20 wt%.

**Table S6** Summary of photophysical data of binary and ternary TSF films.

| Fluorophore | Composition[a] | $\lambda_{em}$[b] [nm] | FWHM [nm] | τ[b] [ns] | PLQY [%] |
| --- | --- | --- | --- | --- | --- |
| ICz-2 | PPF: 1 wt% | 454 | 17 | 2.8 | 14.6 |
| | PPF: CzBPCN: 1 wt% | 454 | 26 | 1163.8 | 32.1 |
| | PPF: CzBPCN: 2 wt% | 453 | 22 | 860.6 | 25.8 |
| | PPF: CzBPCN: 3 wt% | 454 | 22 | 620.5 | 22.2 |
| ICz-3 | mCBCP: 1 wt% | 518 | 27 | 2.9 | 17.7 |
| | mCBCP: 4TCzIPN: 1 wt% | 520 | 32 | 2591.4 | 42.3 |
| | mCBCP: 4TCzIPN: 2 wt% | 519 | 29 | 1767.0 | 36.7 |
| | mCBCP: 4TCzIPN: 3 wt% | 519 | 28 | 1184.8 | 26.9 |

[a] Weight fraction is the portion of fluorophore in each films. TADF material (CzBPCN/4TCzIPN) was added in the portion of 20 wt%. [b] Measured in 298 K. The films were deposited on pre-cleaned quartz flakes. [c] Measured with an integrating sphere in 298 K.

## Device Fabrication and Characterization

Before device fabrication, the ITO glass was meticulously cleaned. Then the ITO glass substrate was transferred into the system. All the organic materials for device fabrication were sublimed before use. The device was fabricated in vacuum under the pressure of $5\times10^{-6}$ Torr. The organic layers were thermally evaporated at a rate of 1.0 Å $s^{-1}$. After all the organic layers were deposited, 0.5 nm of LiF and 150 nm of aluminum were evaporated at the organic surface. The EL and luminescence spectra were recorded by a PR650 spectrometer. The electronic properties of the devices were measured by a Keithley 2400 source meter. All the measurements of devices were performed on common lab conditions.

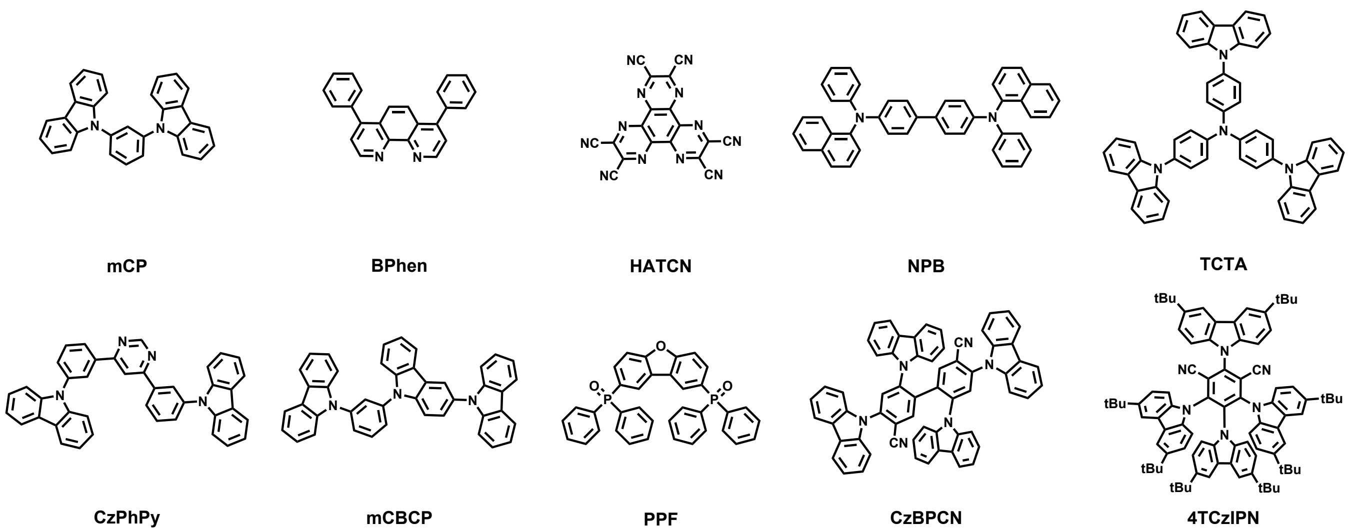



**Fig. S32** The molecule structures of organic materials used in device fabrication.

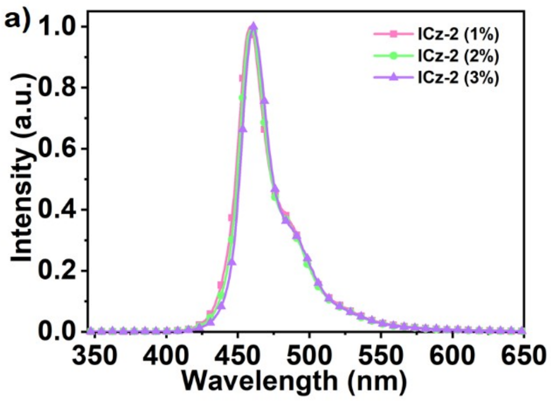



**Fig. S33** The EL spectra of a) device B and b) device G with different fluorophore doping concentrations.

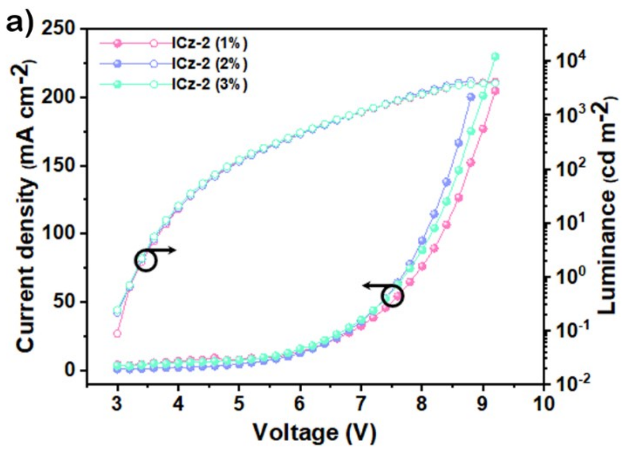



**Fig. S34** The *J-V-L* curves of a) device B and b) device G with different fluorophore doping concentrations.

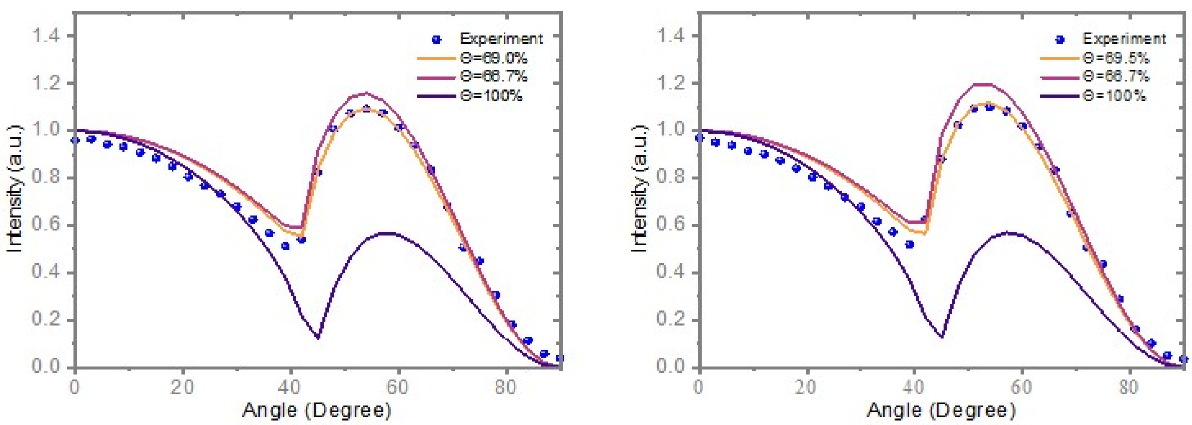



**Fig. S35** Experimentally obtained angle-dependent PL emission of PPF: CzBPCN (20 wt %): ICz-2 (1 wt%) **(Left)** and mCBCP: 4TCzIPN (20 wt%): ICz-3 (1 wt%) (**Right**) films on silica substrate (dots) compared to the simulated curves (lines) with a different ratios of horizontal dipoles (Θ) (violet line for Θ = 100% (fully horizontal), orange lines for Θ = 69.0% and 69.5% for ICz-2 and ICz-3, respectively, and purple line for Θ = 66.7% (isotropic)).

**Table S7** Summary of electroluminescent properties of device B and device G

| Device | Fluorophore Doping Concentration [% in wt] | $\lambda_{EL}$ [nm] | FWHM [nm] | $EQE_{max}$ [%] | $CE_{max}$ [cd/A] | $PE_{max}$ [lm/W] | $V_{on}$ [V] |
|---|---|---|---|---|---|---|---|
| Device B | 1 | 459 | 25 | 3.8 | 35.0 | 60.3 | 3.4 |
| | 2 | 460 | 25 | 3.5 | 34.6 | 55.5 | 3.4 |
| | 3 | 460 | 25 | 3.2 | 31.3 | 51.2 | 3.3 |
| Device G | 1 | 531 | 21 | 12.5 | 86.7 | 106.1 | 3.0 |
| | 2 | 532 | 21 | 12.2 | 82.5 | 92.3 | 3.0 |
| | 3 | 532 | 22 | 9.5 | 69.7 | 77.2 | 3.0 |

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## Cartesian Coordinates:

**ICz ($S_0$):**

| | | | |
|---|---|---|---|
| C | 0.00000100 | 3.50892800 | 0.00034300 |
| C | 1.24824600 | 2.84987800 | 0.00012700 |
| C | 1.26348300 | 1.44783700 | -0.00057100 |
| C | 0.00000100 | 0.87789600 | -0.00123000 |
| C | -1.26348200 | 1.44783700 | -0.00054300 |
| C | -1.24824500 | 2.84987700 | 0.00014700 |
| N | 0.00000000 | -0.48922400 | -0.00141900 |
| C | -1.34176500 | -0.89982600 | -0.00063600 |
| C | -2.16214000 | 0.28543900 | -0.00007900 |
| C | -1.89496400 | -2.17482100 | -0.00044900 |
| C | -3.28831400 | -2.27900000 | 0.00041000 |
| C | -4.10508000 | -1.14023400 | 0.00097200 |
| C | -3.54943300 | 0.14080200 | 0.00072200 |
| C | 1.34176600 | -0.89982500 | -0.00058700 |
| C | 2.16214000 | 0.28543900 | -0.00016800 |
| C | 3.54943500 | 0.14080100 | 0.00061800 |
| C | 4.10507900 | -1.14023500 | 0.00100000 |
| C | 3.28831200 | -2.27900200 | 0.00057700 |
| C | 1.89496300 | -2.17482200 | -0.00026300 |
| H | 0.00000000 | 4.59529900 | 0.00091900 |
| H | 2.16226200 | 3.43651800 | 0.00067600 |
| H | -2.16226000 | 3.43651900 | 0.00074400 |
| H | -1.26778400 | -3.06004300 | -0.00087700 |
| H | -3.74393300 | -3.26494300 | 0.00064200 |
| H | -5.18477300 | -1.25628300 | 0.00159000 |
| H | -4.18966000 | 1.01847500 | 0.00108700 |
| H | 4.18966100 | 1.01847400 | 0.00089700 |
| H | 5.18477200 | -1.25628700 | 0.00162200 |
| H | 3.74393200 | -3.26494400 | 0.00090100 |
| H | 1.26777900 | -3.06004100 | -0.00061100 |

**ICz ($S_1$):**

| | | | |
|---|---|---|---|
| C | 0.00000000 | 3.53948100 | 0.00012500 |
| C | 1.25574400 | 2.90040300 | 0.00007200 |
| C | 1.26426900 | 1.46382600 | -0.00009300 |
| C | 0.00000000 | 0.92061600 | -0.00019400 |
| C | -1.26426900 | 1.46382600 | -0.00008500 |
| C | -1.25574300 | 2.90040300 | 0.00008000 |
| N | 0.00000000 | -0.49856500 | -0.00023200 |
| C | -1.31367200 | -0.90683400 | -0.00015900 |
| C | -2.14139600 | 0.30942500 | 0.00001000 |
| C | -1.85244300 | -2.19615400 | -0.00019900 |
| C | -3.23949200 | -2.32287700 | -0.00002100 |
| C | -4.05490500 | -1.16888600 | 0.00017300 |
| C | -3.52650000 | 0.12879500 | 0.00018100 |
| C | 1.31367200 | -0.90683400 | -0.00013800 |
| C | 2.14139600 | 0.30942500 | 0.00000700 |

| | | | |
|---|---|---|---|
| C | 3.52650000 | 0.12879500 | 0.00017100 |
| C | 4.05490500 | -1.16888600 | 0.00019500 |
| C | 3.23949200 | -2.32287700 | 0.00005400 |
| C | 1.85244300 | -2.19615400 | -0.00012000 |
| H | 0.00000000 | 4.62775400 | 0.00026100 |
| H | 2.16880500 | 3.48482800 | 0.00014600 |
| H | -2.16880500 | 3.48482800 | 0.00016200 |
| H | -1.20474800 | -3.06681600 | -0.00034200 |
| H | -3.69523400 | -3.30683200 | -0.00003100 |
| H | -5.13420500 | -1.29287100 | 0.00030300 |
| H | -4.19202000 | 0.98631100 | 0.00030500 |
| H | 4.19202000 | 0.98631100 | 0.00026700 |
| H | 5.13420500 | -1.29287100 | 0.00031800 |
| H | 3.69523400 | -3.30683200 | 0.00008500 |
| H | 1.20474800 | -3.06681600 | -0.00020000 |

**ICz-2 ($S_0$):**

| | | | |
|---|---|---|---|
| C | -0.00354100 | 4.13275700 | 0.09541600 |
| C | 1.23293200 | 3.47302900 | -0.11591800 |
| C | 1.25983100 | 2.15180900 | -0.58298500 |
| C | -0.00418700 | 1.62080300 | -0.80938400 |
| C | -1.26451800 | 2.15543400 | -0.58771200 |
| C | -1.23772000 | 3.48256100 | -0.12185700 |
| N | -0.00514900 | 0.27428900 | -1.04281900 |
| C | -1.33570000 | -0.15519800 | -0.95259300 |
| C | -2.17046500 | 0.99689700 | -0.74361800 |
| C | -1.83123000 | -1.44263900 | -1.00309000 |
| C | -3.19602700 | -1.65836200 | -0.76633100 |
| C | -4.05567100 | -0.54055200 | -0.53871300 |
| C | -3.56243400 | 0.79736600 | -0.63671700 |
| C | 1.32449100 | -0.15894300 | -0.94880000 |
| C | 2.16254200 | 0.98997700 | -0.73917700 |
| C | 3.55350900 | 0.78778000 | -0.63234200 |
| C | 4.04364100 | -0.55141000 | -0.53349400 |
| C | 3.18071000 | -1.66692800 | -0.75877300 |
| C | 1.81638900 | -1.44773300 | -0.99667500 |
| C | 0.04463800 | 5.58783900 | 0.60173300 |
| C | 0.82946900 | 6.45419100 | -0.40734800 |
| C | -1.35472400 | 6.20378400 | 0.76649900 |
| C | 0.75168200 | 5.63477200 | 1.97332100 |
| C | 5.40609800 | -0.77916300 | -0.10656400 |
| C | 6.26072300 | 0.31834600 | 0.20132700 |
| C | 7.50129100 | 0.07291800 | 0.79594600 |
| C | 7.96174700 | -1.21894700 | 1.06558100 |
| C | 7.14659600 | -2.28516400 | 0.69253500 |
| C | 5.88645300 | -2.10004200 | 0.10328500 |

| | | | |
|---|---|---|---|
| C | 4.51815600 | 1.88574700 | -0.63424600 |
| C | 5.84091300 | 1.66928000 | -0.17201500 |
| C | 5.06083100 | -3.23995400 | -0.29858700 |
| C | 3.72849900 | -3.02363200 | -0.73466600 |
| C | 4.18859900 | 3.14473900 | -1.17705900 |
| C | 5.09042400 | 4.19520200 | -1.17302600 |
| C | 6.37151100 | 4.00506700 | -0.63890700 |
| C | 6.74051400 | 2.75581800 | -0.16887700 |
| C | 5.56144000 | -4.55974600 | -0.28578100 |
| C | 4.78594900 | -5.63551800 | -0.67989400 |
| C | 3.47192600 | -5.42105000 | -1.11655800 |
| C | 2.96139400 | -4.13585200 | -1.14479700 |
| C | -5.41813300 | -0.76556300 | -0.10997200 |
| C | -6.26931000 | 0.33358200 | 0.20155000 |
| C | -5.84683000 | 1.68391300 | -0.17066000 |
| C | -4.52457300 | 1.89733500 | -0.63591000 |
| C | -3.74790500 | -3.01347200 | -0.74527900 |
| C | -5.08008100 | -3.22697900 | -0.30748800 |
| C | -5.90152200 | -2.08554200 | 0.09876800 |
| C | -6.74316500 | 2.77307600 | -0.16303600 |
| C | -6.37147400 | 4.02231600 | -0.63105800 |
| C | -5.09130400 | 4.20962100 | -1.16825200 |
| C | -4.19300200 | 3.15620900 | -1.17755900 |
| C | -2.98508900 | -4.12682500 | -1.16021700 |
| C | -3.49954000 | -5.41056700 | -1.13464800 |
| C | -4.81335000 | -5.62229400 | -0.69605200 |
| C | -5.58478600 | -4.54519000 | -0.29750600 |
| C | -7.16055900 | -2.26844200 | 0.69096400 |
| C | -7.97204100 | -1.20070000 | 1.06783100 |
| C | -7.50908300 | 0.09035900 | 0.79887800 |
| C | -9.33358400 | -1.39249800 | 1.75080300 |
| C | -9.68217400 | -2.87527800 | 1.95621300 |
| C | -9.31008200 | -0.70593100 | 3.13312200 |
| C | -10.43692300 | -0.75334400 | 0.88057000 |
| C | 9.32469400 | -1.41317500 | 1.74504200 |
| C | 9.30674500 | -0.72461000 | 3.12644200 |
| C | 9.67016300 | -2.89653900 | 1.95152000 |
| C | 10.42717100 | -0.77798900 | 0.87080400 |
| H | 2.14974600 | 3.99370400 | 0.12665800 |
| H | -2.15600000 | 4.00054900 | 0.11045500 |
| H | -1.15247500 | -2.26971900 | -1.15578800 |
| H | 1.13534000 | -2.27308600 | -1.14821900 |
| H | 0.35083300 | 6.43655700 | -1.39336100 |
| H | 1.86028100 | 6.10551700 | -0.52967700 |
| H | 0.86923400 | 7.49610700 | -0.06686600 |
| H | -1.91147700 | 6.21376500 | -0.17754700 |

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|---|---|---|---|
| H | -1.26003600 | 7.24135600 | 1.10566200 |
| H | -1.95408100 | 5.66838700 | 1.51113000 |
| H | 1.77882100 | 5.25998800 | 1.91694000 |
| H | 0.21397900 | 5.02698000 | 2.70989400 |
| H | 0.79336300 | 6.66527600 | 2.34690200 |
| H | 8.12526300 | 0.91281900 | 1.07378400 |
| H | 7.48484700 | -3.29152300 | 0.89004100 |
| H | 3.22294500 | 3.27918200 | -1.64431900 |
| H | 4.81013100 | 5.15166300 | -1.60510700 |
| H | 7.08962000 | 4.82006500 | -0.63023500 |
| H | 7.75972800 | 2.60995100 | 0.16907200 |
| H | 6.58500400 | -4.74494700 | 0.01681500 |
| H | 5.20254000 | -6.63851100 | -0.66369400 |
| H | 2.85852000 | -6.25531000 | -1.44447900 |
| H | 1.95431000 | -3.99005900 | -1.51692900 |
| H | -7.76191800 | 2.62955600 | 0.17734300 |
| H | -7.08685400 | 4.83965900 | -0.61822800 |
| H | -4.80859000 | 5.16654200 | -1.59761100 |
| H | -3.22847700 | 3.28803700 | -1.64780900 |
| H | -1.97840300 | -3.98289700 | -1.53423900 |
| H | -2.88939500 | -6.24574200 | -1.46633500 |
| H | -5.23303000 | -6.62403400 | -0.68199600 |
| H | -6.60845900 | -4.72791600 | 0.00627500 |
| H | -7.50072000 | -3.27430800 | 0.88781700 |
| H | -8.13022600 | 0.93144400 | 1.07949800 |
| H | -8.95008700 | -3.38173100 | 2.59529200 |
| H | -9.74098400 | -3.41627800 | 1.00493300 |
| H | -10.65956100 | -2.95906200 | 2.44414500 |
| H | -8.53476800 | -1.14194300 | 3.77331300 |
| H | -10.27675600 | -0.82905600 | 3.63635300 |
| H | -9.11110200 | 0.36771800 | 3.05175000 |
| H | -10.47401100 | -1.22049800 | -0.11016400 |
| H | -10.27393300 | 0.32000000 | 0.73795900 |
| H | -11.41765000 | -0.88104300 | 1.35455300 |
| H | 8.53222400 | -1.15786300 | 3.76945600 |
| H | 9.11011700 | 0.34940400 | 3.04413200 |
| H | 10.27455000 | -0.84935500 | 3.62708200 |
| H | 8.93872200 | -3.40025100 | 2.59350000 |
| H | 10.64878000 | -2.98208300 | 2.43666000 |
| H | 9.72478800 | -3.43901800 | 1.00083300 |
| H | 10.26656300 | 0.29559500 | 0.72727900 |
| H | 10.46023300 | -1.24652800 | -0.11941500 |
| H | 11.40890100 | -0.90759900 | 1.34216600 |

**ICz-2 ($S_1$):**

| | | | |
|---|---|---|---|
| C | -0.01074500 | 4.11678800 | 0.24193700 |
| C | 1.24091500 | 3.46608900 | 0.04329100 |

| | | | |
|---|---|---|---|
| C | 1.27472100 | 2.12394800 | -0.38669600 |
| C | -0.00419900 | 1.58422600 | -0.57235400 |
| C | -1.28189200 | 2.12477700 | -0.39086100 |
| C | -1.25446600 | 3.47436600 | 0.03846100 |
| N | -0.00407500 | 0.25207500 | -0.80623100 |
| C | -1.34435600 | -0.17630400 | -0.78017700 |
| C | -2.17215100 | 0.99233100 | -0.59074800 |
| C | -1.83265200 | -1.45547800 | -0.82702700 |
| C | -3.22240500 | -1.67775000 | -0.62545800 |
| C | -4.08189200 | -0.55418900 | -0.45172200 |
| C | -3.58161200 | 0.79078500 | -0.55048500 |
| C | 1.33685600 | -0.17835900 | -0.78065900 |
| C | 2.16524900 | 0.98885300 | -0.58837600 |
| C | 3.57352400 | 0.78622200 | -0.54781600 |
| C | 4.07198700 | -0.55932400 | -0.45624700 |
| C | 3.21124200 | -1.68254600 | -0.63581600 |
| C | 1.82267400 | -1.45826800 | -0.83624300 |
| C | 0.03508100 | 5.58047500 | 0.71665800 |
| C | 0.81611200 | 6.42645000 | -0.31404300 |
| C | -1.36177800 | 6.20339900 | 0.87727100 |
| C | 0.74973800 | 5.65412400 | 2.08432700 |
| C | 5.45625800 | -0.77634300 | -0.11588700 |
| C | 6.33133900 | 0.32836800 | 0.10809900 |
| C | 7.61167300 | 0.09187500 | 0.61509800 |
| C | 8.09382200 | -1.19807400 | 0.87300700 |
| C | 7.25973700 | -2.27023400 | 0.57883200 |
| C | 5.95529900 | -2.09732300 | 0.07663600 |
| C | 4.52391900 | 1.87483900 | -0.62593900 |
| C | 5.88356600 | 1.67034500 | -0.25357000 |
| C | 5.11143500 | -3.24087700 | -0.24518500 |
| C | 3.74626200 | -3.02735200 | -0.60138500 |
| C | 4.15013000 | 3.13667200 | -1.14896000 |
| C | 5.04408200 | 4.18837800 | -1.21278500 |
| C | 6.36317500 | 4.00775600 | -0.76846000 |
| C | 6.77162600 | 2.76219200 | -0.31889900 |
| C | 5.60952600 | -4.56233300 | -0.22859800 |
| C | 4.80895800 | -5.64717700 | -0.53425100 |
| C | 3.46290600 | -5.43962500 | -0.87851100 |
| C | 2.95022500 | -4.15862900 | -0.91328200 |
| C | -5.46626500 | -0.76808400 | -0.11205000 |
| C | -6.34050200 | 0.33829100 | 0.10455600 |
| C | -5.89052500 | 1.67815200 | -0.26182900 |
| C | -4.53000800 | 1.87922800 | -0.63514300 |
| C | -3.75708100 | -3.02181100 | -0.58368500 |
| C | -5.12322800 | -3.23267700 | -0.22698400 |
| C | -5.96646700 | -2.08759300 | 0.08632000 |

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|---|---|---|---|
| C | -6.77544800 | 2.77214200 | -0.32882700 |
| C | -6.36333300 | 4.01550500 | -0.78126900 |
| C | -5.04431200 | 4.19221000 | -1.22765400 |
| C | -4.15332800 | 3.13854000 | -1.16279400 |
| C | -2.96065600 | -4.15492400 | -0.88870400 |
| C | -3.47373300 | -5.43509500 | -0.84626800 |
| C | -4.82034400 | -5.64021600 | -0.50096600 |
| C | -5.62137500 | -4.55434400 | -0.20224300 |
| C | -7.27304500 | -2.25705800 | 0.58636000 |
| C | -8.10685500 | -1.18328200 | 0.87237800 |
| C | -7.62238900 | 0.10529000 | 0.60885800 |
| C | -9.51781500 | -1.35720600 | 1.45011500 |
| C | -9.88117300 | -2.83379300 | 1.67300000 |
| C | -9.60497700 | -0.62720200 | 2.80760200 |
| C | -10.54715400 | -0.74821300 | 0.47375900 |
| C | 9.50280400 | -1.37678900 | 1.45446200 |
| C | 9.58553900 | -0.65659800 | 2.81744700 |
| C | 9.86508000 | -2.85502300 | 1.66832200 |
| C | 10.53619500 | -0.76145600 | 0.48641200 |
| H | 2.15196200 | 4.00288300 | 0.26576800 |
| H | -2.16987200 | 4.00358600 | 0.24978800 |
| H | -1.15006200 | -2.28485600 | -0.94301700 |
| H | 1.13926400 | -2.28591100 | -0.96027300 |
| H | 0.33251400 | 6.38805100 | -1.29695500 |
| H | 1.84654500 | 6.07761800 | -0.43378200 |
| H | 0.85296200 | 7.47480600 | 0.00653500 |
| H | -1.92331700 | 6.19669900 | -0.06365300 |
| H | -1.26164400 | 7.24683600 | 1.19631200 |
| H | -1.95760900 | 5.68318300 | 1.63512100 |
| H | 1.77777000 | 5.28296000 | 2.03033700 |
| H | 0.21713300 | 5.05813800 | 2.83402800 |
| H | 0.78642300 | 6.69212400 | 2.43722000 |
| H | 8.25394500 | 0.93581100 | 0.83152700 |
| H | 7.61354000 | -3.27227800 | 0.76873400 |
| H | 3.15325700 | 3.26437200 | -1.54674600 |
| H | 4.73013900 | 5.14161800 | -1.62875500 |
| H | 7.07536900 | 4.82659800 | -0.81441100 |
| H | 7.81277000 | 2.62628300 | -0.05012400 |
| H | 6.65161400 | -4.74162600 | 0.00730100 |
| H | 5.22354400 | -6.65078100 | -0.51821000 |
| H | 2.82612300 | -6.28337500 | -1.12930500 |
| H | 1.91570100 | -4.02761200 | -1.20723800 |
| H | -7.81659300 | 2.64055900 | -0.05822500 |
| H | -7.07315800 | 4.83632400 | -0.82769700 |
| H | -4.72816700 | 5.14410000 | -1.64466700 |
| H | -3.15671300 | 3.26179700 | -1.56243900 |

| | | | |
|---|---|---|---|
| H | -1.92603400 | -4.02595500 | -1.18283800 |
| H | -2.83730700 | -6.28063700 | -1.09147600 |
| H | -5.23453700 | -6.64382600 | -0.47877000 |
| H | -6.66338600 | -4.73257200 | 0.03445900 |
| H | -7.62789400 | -3.25784800 | 0.78064100 |
| H | -8.26498400 | 0.95059100 | 0.81859200 |
| H | -9.20190600 | -3.31825800 | 2.38343800 |
| H | -9.86452700 | -3.40393600 | 0.73723000 |
| H | -10.89413400 | -2.90481700 | 2.08421100 |
| H | -8.88194200 | -1.03915200 | 3.52066900 |
| H | -10.60832900 | -0.74009700 | 3.23563400 |
| H | -9.40400100 | 0.44466500 | 2.70911100 |
| H | -10.50592400 | -1.24814600 | -0.50062500 |
| H | -10.37243300 | 0.32009800 | 0.30917900 |
| H | -11.56233900 | -0.86180700 | 0.87263200 |
| H | 8.85994500 | -1.07361100 | 3.52497100 |
| H | 9.38462600 | 0.41586900 | 2.72581300 |
| H | 10.58739900 | -0.77247800 | 3.24832800 |
| H | 9.18328500 | -3.34420300 | 2.37307800 |
| H | 10.87671100 | -2.92931900 | 2.08235300 |
| H | 9.85113200 | -3.41866300 | 0.72858000 |
| H | 10.36275700 | 0.30813000 | 0.32903500 |
| H | 10.49793900 | -1.25410500 | -0.49180700 |
| H | 11.54999300 | -0.87874900 | 0.88789300 |

**ICz-3 ($S_0$):**

| | | | |
|---|---|---|---|
| C | -1.25727800 | 2.07616200 | 0.45755300 |
| C | 0.01973200 | 2.74362900 | 0.49581700 |
| C | 1.28490400 | 2.05345200 | 0.45517300 |
| C | 1.27674300 | 0.67490500 | 0.12051500 |
| C | -0.00383300 | 0.13634900 | 0.04094700 |
| C | -1.27434000 | 0.69723800 | 0.12187300 |
| C | 2.49907500 | 4.20440200 | 0.74405900 |
| C | 2.47757700 | 2.79158100 | 0.84327700 |
| C | -2.43521800 | 2.83524100 | 0.84718700 |
| C | -2.43047900 | 4.24880300 | 0.74905400 |
| C | -1.18138600 | 4.93176100 | 0.42353100 |
| C | 0.03221000 | 4.19396300 | 0.48494800 |
| C | -3.57117300 | 2.18880800 | 1.37533500 |
| C | -4.71348200 | 2.89692200 | 1.70216300 |
| C | -4.74453600 | 4.28480000 | 1.51093300 |
| C | -3.61356200 | 4.94833700 | 1.06186300 |
| C | 3.69351400 | 4.88289700 | 1.05760300 |
| C | 4.81292400 | 4.19941500 | 1.50657300 |
| C | 4.75672800 | 2.81261900 | 1.69797900 |
| C | 3.60133900 | 2.12510400 | 1.37198500 |
| C | -1.14331000 | 6.30223900 | 0.12732300 |

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|---|---|---|---|
| C | 0.05466900 | 6.99016800 | -0.05953200 |
| C | 1.24398700 | 6.27626800 | 0.12180100 |
| C | 1.26183200 | 4.91057900 | 0.41834900 |
| N | -0.01594500 | -1.22006000 | -0.10094000 |
| C | -2.17473800 | -0.45199700 | -0.13051100 |
| C | -1.34924500 | -1.63131900 | -0.15076600 |
| C | 2.15649800 | -0.49068500 | -0.13160100 |
| C | 1.30990500 | -1.65567500 | -0.15059200 |
| C | -3.54708700 | -0.63419800 | -0.41776300 |
| C | -4.09603300 | -1.95150600 | -0.31770800 |
| C | -3.24957600 | -3.09417700 | -0.20403300 |
| C | -1.85811000 | -2.91279100 | -0.19720000 |
| C | -6.10665600 | -3.39289900 | -0.03558400 |
| C | -5.24765500 | -4.57953300 | -0.03422800 |
| C | -3.83915900 | -4.43102800 | -0.12368300 |
| C | -4.41690800 | 0.43710200 | -0.88735900 |
| C | -5.53142900 | -2.11149800 | -0.26810400 |
| C | -5.78598500 | -5.88237600 | 0.03508900 |
| C | -4.97809200 | -7.00543500 | 0.03094500 |
| C | -3.58703800 | -6.85874300 | -0.04846200 |
| C | -3.03615400 | -5.59259000 | -0.12613900 |
| C | -6.38963200 | -0.98202600 | -0.37063400 |
| C | -7.76226100 | -1.13557800 | -0.13107400 |
| C | -8.32980000 | -2.37248300 | 0.16799100 |
| C | -7.48447000 | -3.48536700 | 0.18932400 |
| C | 0.11096800 | 8.47995100 | -0.42466500 |
| C | -1.28780900 | 9.09663300 | -0.58293800 |
| C | 0.85644300 | 9.25055800 | 0.68602100 |
| C | 0.86779500 | 8.64789800 | -1.75938900 |
| C | -9.82637700 | -2.55277700 | 0.45983300 |
| C | -10.60066500 | -1.22716400 | 0.38728600 |
| C | -10.43475600 | -3.52510300 | -0.57335300 |
| C | -10.00111400 | -3.13776300 | 1.87766300 |
| C | 3.52447500 | -0.69683900 | -0.41940600 |
| C | 4.05058800 | -2.02355200 | -0.31832400 |
| C | 1.79582700 | -2.94558300 | -0.19666700 |
| C | -5.82460200 | 0.29580800 | -0.80053200 |
| C | -3.88272700 | 1.58841100 | -1.50176400 |
| C | -4.69653400 | 2.62332500 | -1.92474700 |
| C | -6.08228500 | 2.52944900 | -1.74411600 |
| C | -6.63344200 | 1.37523500 | -1.21116800 |
| C | 4.41248200 | 0.35951900 | -0.89107900 |
| C | 5.81711200 | 0.19571500 | -0.80353300 |
| C | 6.36127800 | -1.09054000 | -0.36848300 |
| C | 5.48289600 | -2.20840500 | -0.26613100 |
| C | 5.15822200 | -4.66744900 | -0.02789500 |

| | | | |
|---|---|---|---|
| C | 3.75191300 | -4.49654500 | -0.12033000 |
| C | 3.18471600 | -3.15109200 | -0.20339100 |
| C | 3.89736300 | 1.51780700 | -1.50802700 |
| C | 4.72831800 | 2.53839100 | -1.93320600 |
| C | 6.11216900 | 2.42170700 | -1.75330800 |
| C | 6.64390900 | 1.25929900 | -1.21776100 |
| C | 5.67489200 | -5.97936400 | 0.04548200 |
| C | 4.84866400 | -7.08870800 | 0.04197500 |
| C | 3.46007000 | -6.91962200 | -0.04062700 |
| C | 2.93006300 | -5.64506200 | -0.12196100 |
| C | 7.72497400 | -1.26928800 | -0.12500800 |
| C | 8.27473500 | -2.51839500 | 0.17956900 |
| C | 7.41559900 | -3.61455700 | 0.20046700 |
| C | 6.03559300 | -3.49560600 | -0.03037200 |
| C | 9.77912700 | -2.63607000 | 0.46249600 |
| C | 10.56927000 | -2.16550000 | -0.77740300 |
| C | 10.14164000 | -1.74420700 | 1.66907400 |
| C | 10.20415300 | -4.07741700 | 0.78512700 |
| H | -3.53625600 | 1.11998600 | 1.54039300 |
| H | -5.57831000 | 2.37623800 | 2.10130300 |
| H | -5.64031000 | 4.84965600 | 1.75329500 |
| H | -3.63226400 | 6.03067300 | 0.99946300 |
| H | 3.73056500 | 5.96483300 | 0.99610800 |
| H | 5.71850600 | 4.74830000 | 1.74913600 |
| H | 5.61194400 | 2.27634000 | 2.09719500 |
| H | 3.54717400 | 1.05723300 | 1.53799700 |
| H | -2.07951700 | 6.83292500 | 0.02418100 |
| H | 2.18730000 | 6.79764500 | 0.01244600 |
| H | -1.18046000 | -3.75426300 | -0.18337900 |
| H | -6.85968400 | -6.02067300 | 0.07260700 |
| H | -5.42449200 | -7.99438300 | 0.08069900 |
| H | -2.94144800 | -7.73223000 | -0.05748800 |
| H | -1.95902500 | -5.50506400 | -0.20088100 |
| H | -8.39652600 | -0.26154300 | -0.16972300 |
| H | -7.91778400 | -4.45115100 | 0.41387400 |
| H | -1.86549600 | 9.04192200 | 0.34669800 |
| H | -1.86329100 | 8.60356400 | -1.37453600 |
| H | -1.19543500 | 10.15483300 | -0.85151500 |
| H | 0.34290100 | 9.14418800 | 1.64832200 |
| H | 0.90615300 | 10.31868000 | 0.44200400 |
| H | 1.88253600 | 8.89010700 | 0.81320300 |
| H | 0.35876300 | 8.11139000 | -2.56823300 |
| H | 1.89176800 | 8.26507200 | -1.69696200 |
| H | 0.92374400 | 9.70780200 | -2.03578500 |
| H | -10.54215300 | -0.77439100 | -0.60900500 |
| H | -10.23155900 | -0.49884000 | 1.11819500 |

| | | | |
|---|---|---|---|
| H | -11.65906500 | -1.40695000 | 0.60606100 |
| H | -10.32365900 | -3.13435400 | -1.59123900 |
| H | -11.50433500 | -3.66885300 | -0.37804000 |
| H | -9.95497300 | -4.50881000 | -0.53900900 |
| H | -9.57868300 | -2.46545700 | 2.63310800 |
| H | -9.50641700 | -4.10917100 | 1.98116400 |
| H | -11.06500000 | -3.27911200 | 2.10356700 |
| H | 1.10365800 | -3.77522200 | -0.18211100 |
| H | -2.81341600 | 1.65422800 | -1.65266900 |
| H | -4.25866100 | 3.50308800 | -2.38613200 |
| H | -6.73149000 | 3.34234700 | -2.05687900 |
| H | -7.71265200 | 1.29438900 | -1.15209200 |
| H | 2.82925300 | 1.60127700 | -1.65877900 |
| H | 4.30491300 | 3.42437200 | -2.39619900 |
| H | 6.77487200 | 3.22263700 | -2.06857400 |
| H | 7.72158900 | 1.15955000 | -1.15925400 |
| H | 6.74603500 | -6.13546000 | 0.08526700 |
| H | 5.27864200 | -8.08476500 | 0.09475400 |
| H | 2.80045300 | -7.78257100 | -0.04921400 |
| H | 1.85469100 | -5.54003600 | -0.19913500 |
| H | 8.38163700 | -0.40909200 | -0.16321500 |
| H | 7.82317600 | -4.58821200 | 0.42849800 |
| H | 10.34465100 | -1.12462600 | -1.03269800 |
| H | 10.33049300 | -2.78270200 | -1.65099400 |
| H | 11.64786200 | -2.23845700 | -0.59260500 |
| H | 9.90502400 | -0.69132200 | 1.48353800 |
| H | 11.21494800 | -1.81173700 | 1.88413100 |
| H | 9.59417100 | -2.05709100 | 2.56545400 |
| H | 10.00237400 | -4.75906700 | -0.04890800 |
| H | 9.69492000 | -4.46316800 | 1.67553100 |
| H | 11.28153400 | -4.10772400 | 0.98188000 |

**ICz-3 ($S_1$):**

| | | | |
|---|---|---|---|
| C | 1.27173400 | 2.07240300 | -0.53341200 |
| C | -0.01453200 | 2.74027800 | -0.55018400 |
| C | -1.29371500 | 2.05209400 | -0.53030400 |
| C | -1.28821200 | 0.65697600 | -0.22478000 |
| C | 0.00129600 | 0.11327700 | -0.18420400 |
| C | 1.28471600 | 0.67556600 | -0.22891600 |
| C | -2.49728500 | 4.20652100 | -0.79646400 |
| C | -2.47746800 | 2.78958700 | -0.89864700 |
| C | 2.44631600 | 2.82740300 | -0.89520800 |
| C | 2.44437500 | 4.24461500 | -0.78865800 |
| C | 1.19597800 | 4.92183000 | -0.46254200 |
| C | -0.02499400 | 4.18152000 | -0.52448300 |
| C | 3.60181500 | 2.18656800 | -1.39768700 |
| C | 4.75100700 | 2.89894500 | -1.68967400 |

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|---|---|---|---|
| C | 4.77814300 | 4.28740600 | -1.49671800 |
| C | 3.63224300 | 4.94590700 | -1.07364000 |
| C | -3.69146400 | 4.88905900 | -1.09267300 |
| C | -4.82599100 | 4.21226200 | -1.52039600 |
| C | -4.77854700 | 2.82398700 | -1.70743200 |
| C | -3.62092200 | 2.12965700 | -1.40557900 |
| C | 1.15639300 | 6.28941900 | -0.15222700 |
| C | -0.04305100 | 6.97413700 | 0.03786100 |
| C | -1.23710600 | 6.26549500 | -0.15365900 |
| C | -1.25930200 | 4.90449000 | -0.46356300 |
| N | 0.01120200 | -1.23049600 | -0.02625600 |
| C | 2.16651200 | -0.45041200 | 0.05490300 |
| C | 1.35010700 | -1.64326600 | 0.06497000 |
| C | -2.15457200 | -0.48403800 | 0.05817700 |
| C | -1.31909600 | -1.66381700 | 0.07065000 |
| C | 3.54033300 | -0.63759400 | 0.37763800 |
| C | 4.09676200 | -1.95875600 | 0.27095600 |
| C | 3.26230400 | -3.10230200 | 0.12859500 |
| C | 1.85579600 | -2.91657600 | 0.10350400 |
| C | 6.11585000 | -3.39236100 | 0.02953400 |
| C | 5.26282100 | -4.57597600 | -0.02902300 |
| C | 3.84672300 | -4.42722600 | 0.02988800 |
| C | 4.38286900 | 0.41998300 | 0.89187600 |
| C | 5.53047700 | -2.11460800 | 0.26807200 |
| C | 5.80325300 | -5.87693200 | -0.12203000 |
| C | 4.99737800 | -6.99951900 | -0.16808300 |
| C | 3.60222200 | -6.85403400 | -0.11793100 |
| C | 3.04579400 | -5.59411300 | -0.01910100 |
| C | 6.38259500 | -0.98671500 | 0.43538200 |
| C | 7.76283800 | -1.13490500 | 0.24743900 |
| C | 8.34498800 | -2.36650600 | -0.05935000 |
| C | 7.50592800 | -3.47789300 | -0.14237500 |
| C | -0.09842000 | 8.45891600 | 0.41763400 |
| C | 1.29957700 | 9.07479100 | 0.58520700 |
| C | -0.84282400 | 9.24073700 | -0.68647900 |
| C | -0.85854200 | 8.61147600 | 1.75288100 |
| C | 9.85294300 | -2.53532800 | -0.29393300 |
| C | 10.61968100 | -1.21048900 | -0.15512600 |
| C | 10.42111400 | -3.53333400 | 0.73770900 |
| C | 10.08681400 | -3.08288200 | -1.71818400 |
| C | -3.52359400 | -0.69150900 | 0.38080600 |
| C | -4.05771200 | -2.02253400 | 0.28453000 |
| C | -1.80324300 | -2.94657800 | 0.12372400 |
| C | 5.79886000 | 0.28007600 | 0.86832900 |
| C | 3.82084000 | 1.57305600 | 1.48905800 |
| C | 4.61530800 | 2.60122700 | 1.95690500 |

| | | | |
|---|---|---|---|
| C | 6.00939900 | 2.50445300 | 1.84509600 |
| C | 6.58529200 | 1.35367900 | 1.32793500 |
| C | -4.38646300 | 0.35775000 | 0.88354700 |
| C | -5.79872300 | 0.19688900 | 0.85192200 |
| C | -6.36078100 | -1.08293900 | 0.42437900 |
| C | -5.48846200 | -2.20221200 | 0.27531400 |
| C | -5.18191100 | -4.65992400 | 0.00528700 |
| C | -3.76883900 | -4.48995700 | 0.06821900 |
| C | -3.20400600 | -3.15462900 | 0.15321600 |
| C | -3.84614800 | 1.52186900 | 1.47777000 |
| C | -4.65944100 | 2.54130500 | 1.93442300 |
| C | -6.05045200 | 2.42365700 | 1.81304500 |
| C | -6.60476800 | 1.26020900 | 1.29944800 |
| C | -5.70280600 | -5.97017700 | -0.07535600 |
| C | -4.88029000 | -7.08111400 | -0.10497100 |
| C | -3.48786000 | -6.91430500 | -0.05055400 |
| C | -2.95076600 | -5.64483900 | 0.03596100 |
| C | -7.73123500 | -1.25691900 | 0.22540700 |
| C | -8.29515200 | -2.50405200 | -0.07513200 |
| C | -7.44314700 | -3.60119200 | -0.13797200 |
| C | -6.05212400 | -3.48859800 | 0.04616100 |
| C | -9.80830500 | -2.61212600 | -0.30772000 |
| C | -10.55335200 | -2.15013800 | 0.96307500 |
| C | -10.20642400 | -1.70592600 | -1.49239200 |
| C | -10.25121700 | -4.04799000 | -0.63017000 |
| H | 3.57342300 | 1.11913700 | -1.57263400 |
| H | 5.62612200 | 2.37953200 | -2.06853300 |
| H | 5.67846100 | 4.85422400 | -1.71538100 |
| H | 3.64799800 | 6.02816800 | -1.00534800 |
| H | -3.72247900 | 5.97141300 | -1.02986600 |
| H | -5.73255700 | 4.76586000 | -1.74715600 |
| H | -5.64393800 | 2.29059500 | -2.08909300 |
| H | -3.57541000 | 1.06211900 | -1.57620300 |
| H | 2.09132400 | 6.82032200 | -0.04348700 |
| H | -2.17788500 | 6.79071800 | -0.04464600 |
| H | 1.18104300 | -3.76007200 | 0.06635000 |
| H | 6.87780100 | -6.01337100 | -0.13868800 |
| H | 5.44462000 | -7.98692500 | -0.23473200 |
| H | 2.95863200 | -7.72862300 | -0.14921200 |
| H | 1.96684000 | -5.51130200 | 0.03005200 |
| H | 8.39461800 | -0.26259500 | 0.33313300 |
| H | 7.94891600 | -4.43777100 | -0.37246200 |
| H | 1.87906300 | 9.03044100 | -0.34377700 |
| H | 1.87373300 | 8.57389600 | 1.37274100 |
| H | 1.20535900 | 10.12993000 | 0.86478100 |
| H | -0.32891700 | 9.14308600 | -1.64944100 |

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|---|---|---|---|
| H | -0.88981900 | 10.30628700 | -0.43123600 |
| H | -1.86953800 | 8.88392300 | -0.81723900 |
| H | -0.35102400 | 8.06633300 | 2.55681700 |
| H | -1.88240900 | 8.22990100 | 1.68411300 |
| H | -0.91401600 | 9.66851900 | 2.03992200 |
| H | 10.51879600 | -0.78369100 | 0.84921000 |
| H | 10.27963400 | -0.46414100 | -0.88191900 |
| H | 11.68664400 | -1.38312800 | -0.33423500 |
| H | 10.26626400 | -3.17045200 | 1.76017400 |
| H | 11.49842100 | -3.66851300 | 0.58331400 |
| H | 9.94707100 | -4.51703700 | 0.65665400 |
| H | 9.69242700 | -2.39264700 | -2.47259600 |
| H | 9.60064700 | -4.05278800 | -1.86593500 |
| H | 11.15951700 | -3.21488900 | -1.90435300 |
| H | -1.11369100 | -3.77852900 | 0.09576600 |
| H | 2.74610300 | 1.63688500 | 1.59213700 |
| H | 4.15819000 | 3.47883000 | 2.40350500 |
| H | 6.64389100 | 3.31318600 | 2.19623800 |
| H | 7.66628300 | 1.27412500 | 1.31896300 |
| H | -2.77319400 | 1.60281100 | 1.58737000 |
| H | -4.21814000 | 3.42829800 | 2.37843900 |
| H | -6.69969600 | 3.22483600 | 2.15441000 |
| H | -7.68431200 | 1.16295500 | 1.28380200 |
| H | -6.77507900 | -6.12297300 | -0.09482600 |
| H | -5.31264400 | -8.07575500 | -0.16202100 |
| H | -2.83103900 | -7.77942000 | -0.06876100 |
| H | -1.87337200 | -5.54519100 | 0.08915400 |
| H | -8.38464800 | -0.39647200 | 0.29622400 |
| H | -7.86081700 | -4.57148400 | -0.36117300 |
| H | -10.31520800 | -1.11302800 | 1.22124800 |
| H | -10.28881100 | -2.77762300 | 1.82176600 |
| H | -11.63781700 | -2.21602300 | 0.81359000 |
| H | -9.95944700 | -0.65593000 | -1.30427300 |
| H | -11.28656900 | -1.76717000 | -1.67203600 |
| H | -9.69059100 | -2.01185000 | -2.40966100 |
| H | -10.02544900 | -4.73887500 | 0.18996300 |
| H | -9.77387600 | -4.42709400 | -1.54081900 |
| H | -11.33465500 | -4.07092600 | -0.79131600 |