Supporting Information

Efficient Circularly Polarized Thermally Activated Delayed Fluorescence Hetero-[4]Helicene with Carbonyl-/ Sulfone-Bridged Triarylamine Structures

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1 Experimental Section

1.1 Materials and instruments

All chemicals and reagents were used as received from commercial sources without further purification. tetrahydrofuran and toluene used in synthetic routes were purified by PURE SOLV (Innovative Technology) purification system. ^{1}H NMR and ^{13}C NMR spectra were recorded on a Bruker 400 spectrometer or Bruker 600 spectrometer at room temperature. Mass spectroscopy was performed using a Thermo Fisher ISQ Single Quadrupole GC-MS with direct probe system. Matrix-assisted laser desorption/ionization time-of-flight mass spectrometry (MALDI-TOF-MS) was performed on Bruker Autoflex II/Compass 1.0. Elemental analysis was measured using Vario Micro cube. Ultra-violet-visible absorption spectra were measured by a Shimadzu UV-2600 spectrophotometer. Fluorescent and phosphorescent spectra were measured by a Hitachi F-4600 spectrophotometer. Thermogravimetric analysis (TGA) was performed by a METTLER TOLEDO TGA1 under nitrogen atmosphere. The temperature was increased to 700 ^{o}C with a heating rate of 10 ^{o}C/min. Differential scanning calorimetry (DSC) measurements were performed by a METTLER TOLEDO DSC1 under nitrogen atmosphere. The temperature was increased and decreased with a heating or cooling rate of 10 ^{o}C/min. Molecular geometries were extracted in single crystals and performed by Gaussian 09W program package with density functional theory (DFT) with Beck's three-parameter hybrid exchange functional[1, 2] and Lee, and Yang and Parr correlation functional[3] (B3LYP) with 6-31G(d) basic set. Non-covalent

interactions (NCI) of intramolecular interactions analyses were carried out by Multiwfn[4] with reduced density gradient (RDG).[5] The NCI results were plotted via VMD software (version 1.9.3).[6] Cyclic voltammetry (CV) was performed on a CHI 600D electrochemical work station with a scan rate of 100 mV S^{-1} at room temperature under an argon flow, in which a Pt disk, a Pt plate and a Ag/AgCl electrode were used as working electrode, counter electrode and reference electrode in tetra-n-butylammonium hexa-fluorophosphates (*n*-Bu_4NPF_6, 0.1 M) dichloromethane/ *N,N*-dimethylformamide solution, respectively. For calibration, the redox potential of ferrocene/ferrocenium(Fc/Fc^+) was measured under the same conditions. The photoluminescence quantum efficiency (PLQY) was measured using Hamamatsu C9920-02G in nitrogen or air atmosphere. Transient spectra were obtained by using Quantaurus-Tau fluorescence lifetime measurement system (C11367-03, Hamamatsu Photonics Co.) in air or nitrogen atmosphere. The separation of isomers with chiral configurations was performed by chiral high-performance liquid chromatography (HPLC) were separated by IG column which was employed as stationary phase and hexane/dichloromethane/isopropanol (70/20/10) as eluent. The circular dichroism (CD) spectra were measured on a Jasco-1500 circular dichroism spectrometer. The circularly polarized photoluminescence (CPPL) spectra were measured on a Jasco CPL-300 spectrophotometer with “Standard” sensitivity at 200 nm/min scan speed and respond time of 2.0 s employing “slit” mode. The circularly polarized electroluminescence (CPEL) spectra were measured on a JASCO CPPL-300 spectrophotometer with ‘Standard’ sensitivity at 200 nm/min scan speed and respond time of 2.0 s employing

“band” mode.

1.2 Single crystal information

A suitable crystal was selected and it on a 'Bruker APEX-II CCD' diffractometer. The crystal was kept at 100.0 or 173.0 K during data collection. Using Olex2, the structure was solved with the ShelXT structure solution program using Intrinsic Phasing and refined with the ShelXL refinement package using Least Squares minimization. The crystals of **QPO** and **QPO-PhCz** were grown by slow evaporation in $CHCl_2$ and methanol. The X-ray crystallographic coordinates for structure reported in this study have been deposited at the Cambridge Crystallographic Data Centre (CCDC), under deposition number **QPO** (2051469) and **QPO-PhCz** (2051470). These data can be obtained free of charge from The Cambridge Crystallographic Data Centre “http://www.ccdc.cam.ac.uk/data request/cif”.

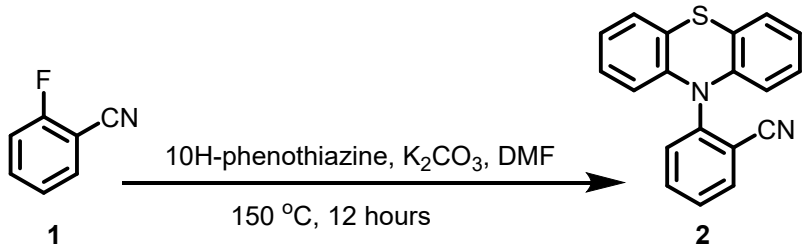
1.3 Device fabrication process

OLEDs were fabricated on ITO glass substrates layer (110 nm, 15 Ω/square) under a base pressure of 3×10^{-6} Torr. The active area of each device is 0.09 cm^2. Deposition rates and thicknesses of all materials were monitored with oscillating quartz crystals. Doping layers were deposited by utilizing two different sensors to monitor the deposition rates of both host material and dopant material. The deposition rate of host was controlled at 0.2 nm s^{-1}, and the deposition rate of the dopant was adjusted according to the volume ratio doped in the host materials. The electroluminescence

(EL) and current density-voltage(*J-V*) characteristics of the devices were measured by a constant current source (Keithley 2400 SourceMeter) combined with a photometer (Photo Research SpectraScan PR655).

1.4 Syntheses of materials

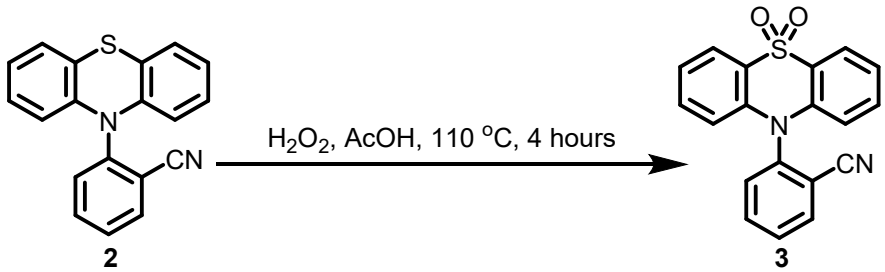
1.4.1 Synthesis of compound **2**



A mixture of **1** (3.0 g, 24.79 mmol), 10*H*-phenothiazine (5.4 g, 27.27 mmol) and aqueous K_2CO_3 (10.0 g, 74.37 mmol) in 100 mL *N*, *N*-Dimethylformamide (DMF) was stirred for 12 hours at 150 °C under a nitrogen atmosphere. After cooled to room temperature, the mixture was extracted with dichloromethane solution (4×30 mL), and the combined organic layer with dichloromethane (DCM) solution was dried over $MgSO_4$. We used rotary evaporation to remove off the solvent and used silica gel column to pass the residue, which using petroleum ether (PE)/ DCM (v/v, 4:1) as an eluent to obtain **2** as white solid (6.8 g, 92%). ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.93 (dd, *J* = 7.7, 1.2 Hz, 1H), 7.87 (td, *J* = 7.9, 1.6 Hz, 1H), 7.68 – 7.59 (m, 2H), 7.08 – 7.01 (m, 2H), 6.90 – 6.80 (m, 4H), 6.07 (dd, *J* = 7.2, 2.2 Hz, 2H). ^{13}C NMR (101 MHz, $CDCl_3$) δ 143.7, 142.8, 135.3, 134.8, 133.5, 129.1, 127.1, 126.9, 123.2, 120.9, 116.2, 115.9, 115.3, 53.4. Anal. calcd for $C_{19}H_{12}N_2S$ (%): C, 75.97; H, 4.03; N, 9.33; S, 10.67; found:

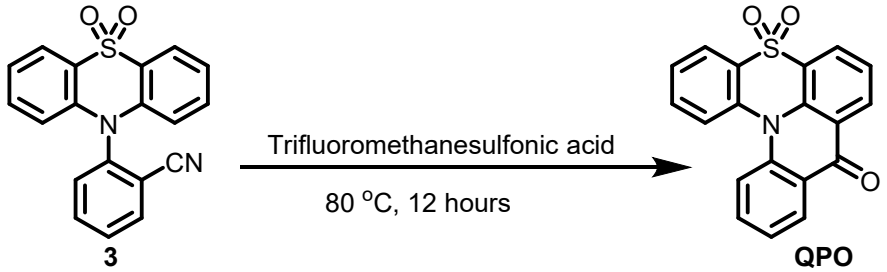
C, 75.84; H, 3.92; N, 9.25; S, 10.62.

1.4.2 Synthesis of compound **3**



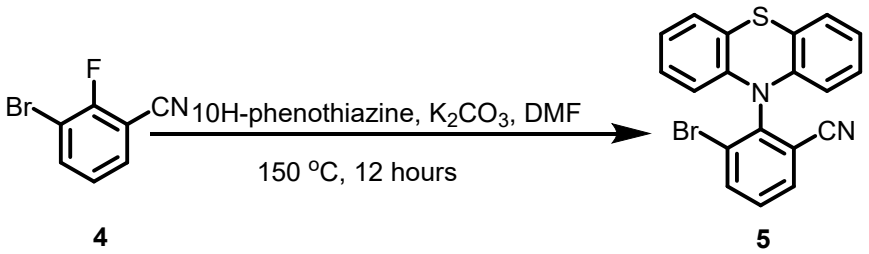
A mixture of **2** (3.0 g, 10.00 mmol) and H_2O_2 (30 wt%, 10 mL) in 50 mL CH_3COOH was stirred for 4 hours at 110 °C under an air atmosphere. After cooled to room temperature, the reaction system was extracted with dichloromethane (4×45 mL), and the combined organic solution was dried over $MgSO_4$. We used rotary evaporation to remove off the solvent and used silica gel column to pass the residue, which using PE/ DCM (v/v, 3:1) as an eluent to obtain **3** as white solid (3.1 g, 95%). ^{1}H NMR (400 MHz, $CDCl_3$) δ 8.21 (dd, *J* = 7.9, 1.5 Hz, 2H), 8.03 (dd, *J* = 7.7, 1.4 Hz, 1H), 7.96 (td, *J* = 7.8, 1.5 Hz, 1H), 7.78 (td, *J* = 7.7, 1.1 Hz, 1H), 7.63 – 7.53 (m, 1H), 7.45 (ddd, *J* = 8.7, 7.3, 1.6 Hz, 2H), 7.36 – 7.28 (m, 2H), 6.47 (d, *J* = 8.5 Hz, 2H). ^{13}C NMR (101 MHz, $CDCl_3$) δ 141.3, 139.7, 136.1, 135.2, 133.2, 132.2, 130.6, 123.9, 123.5, 123.0, 116.3, 115.8, 114.9. Anal. calcd for $C_{19}H_{12}N_2O_2S$ (%): C, 68.66; H, 3.64; N, 8.43; S, 9.65; found: C, 68.63; H, 3.70; N, 8.41; S, 9.76.

1.4.3 Synthesis of compound **QPO**



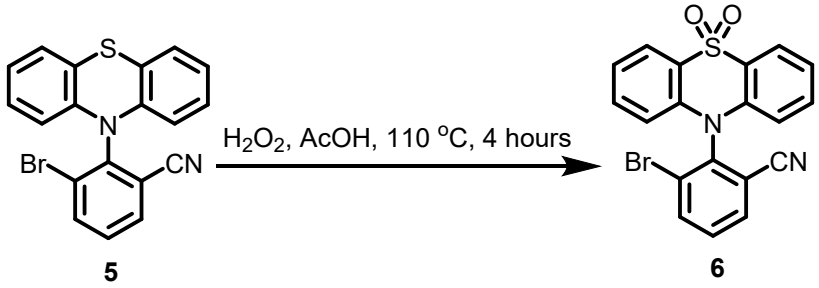
A mixture of **3** (3.0 g, 9.04 mmol) and trifluoromethanesulfonic acid (10 mL) in 50 mL single neck round bottom flask was stirred for 12 hours at 80 °C under an air atmosphere. After cooling to room temperature, the mixture was poured into 100 mL ice water and filtered to get crude product. The crude product was purified by column chromatography on silica gel using PE/ DCM (3/2, v/v) as eluent to afford **QPO** as yellow powder (1.1 g, 35%). ^{1}H NMR (400 MHz, DMSO-d_6) δ 8.56 (dd, J = 7.8, 1.5 Hz, 1H), 8.45 (dd, J = 7.6, 1.5 Hz, 1H), 8.31 (dd, J = 7.9, 1.5 Hz, 1H), 8.19 (dd, J = 7.8, 1.5 Hz, 1H), 8.01 (d, J = 8.5 Hz, 1H), 7.91 – 7.81 (m, 2H), 7.80 – 7.71 (m, 2H), 7.68 – 7.53 (m, 2H). ^{13}C NMR (101 MHz, DMSO-d_6) δ 177.4, 140.2, 139.6, 138.6, 134.5, 133.9, 131.9, 129.2, 128.6, 127.3, 127.1, 126.7, 126.2, 126.1, 125.0, 124.5, 124.2, 123.2, 121.8. MALDI-MS (m/z) of C19H11NO3S for $[M+H]^+$: calcd. 333.05; found, 334.01. Anal. calcd for $C_{19}H_{11}NO_3S$ (%): C, 68.46; H, 3.33; N, 4.20; S, 9.62; found: C, 68.45; H, 3.33; N, 4.31; S, 9.83.

1.4.4 Synthesis of compound **5**



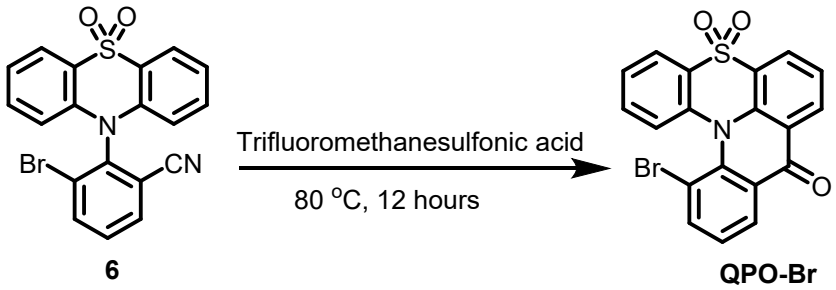
A mixture of **4** (5.0 g, 25.13 mmol), 10*H*-phenothiazine (5.5 g, 27.64 mmol) and aqueous K_2CO_3 (17.3 g, 125.65 mmol) in 100 mL DMF was stirred for 12 hours at 150 °C under a nitrogen atmosphere. After cooled to room temperature, the mixture was extracted with dichloromethane solution (4×30 mL), and the combined organic layer with DCM solution was dried over $MgSO_4$. We used rotary evaporation to remove off the solvent and used silica gel column to pass the residue, which using PE/ DCM (v/v, 1:1) as an eluent to obtain **5** as white solid (8.5 g, 90%). ^{1}H NMR (400 MHz, $CDCl_3$) δ 8.08 (dd, *J* = 8.2, 1.3 Hz, 1H), 7.87 (dd, *J* = 7.7, 1.2 Hz, 1H), 7.49 (t, *J* = 8.0 Hz, 1H), 7.05 – 6.96 (m, 2H), 6.89 – 6.80 (m, 4H), 5.98 – 5.85 (m, 2H). ^{13}C NMR (101 MHz, $CDCl_3$) δ 142.3, 140.2, 139.3, 134.1, 130.4, 128.5, 127.0, 126.9, 123.4, 120.2, 118.7, 115.3, 114.8. Anal. calcd for $C_{19}H_{11}BrN_2S$ (%): C, 60.17; H, 2.92; N, 7.39; S, 8.45; found: C, 60.20; H, 2.96; N, 7.46; S, 8.81.

1.4.5 Synthesis of compound **6**



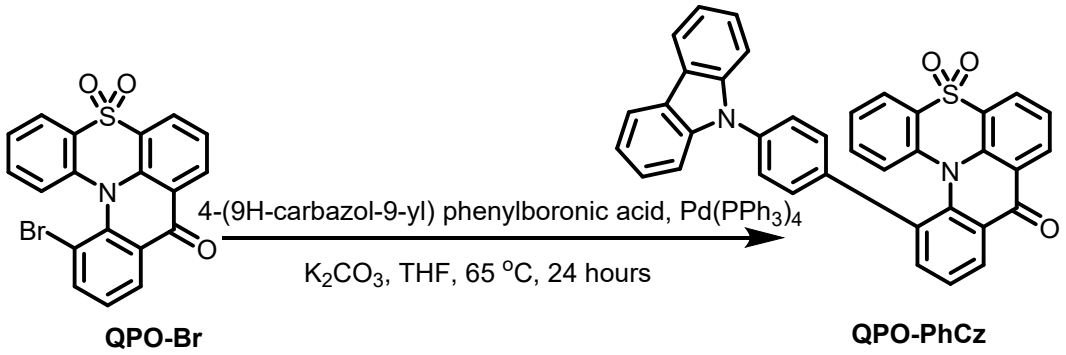
A mixture of **5** (5.0 g, 13.23 mmol) and H_2O_2 (30 wt%, 20 mL) in 100 mL CH_3COOH was stirred for 4 hours at 110 °C under an air atmosphere. After cooled to room temperature, the reaction system was extracted with dichloromethane (4×45 mL), and the combined organic solution was dried over $MgSO_4$. We used rotary evaporation to remove off the solvent and used silica gel column to pass the residue, which using PE/ DCM (v/v, 1:1) as an eluent to obtain **6** as white solid (4.9 g, 91%). ^{1}H NMR (400 MHz, $CDCl_3$) δ 8.24 (dd, J = 7.9, 1.5 Hz, 2H), 8.20 – 8.14 (m, 1H), 8.01 – 7.93 (m, 1H), 7.65 (t, J = 8.0 Hz, 1H), 7.48 (ddd, J = 8.7, 7.3, 1.6 Hz, 2H), 7.35 (t, J = 7.6 Hz, 2H), 6.45 – 6.33 (m, 2H). ^{13}C NMR (101 MHz, $CDCl_3$) δ 139.8, 139.7, 137.9, 134.1, 133.4, 131.7, 127.4, 124.3, 123.8, 123.3, 117.8, 115.4, 114.2. Anal. calcd for $C_{19}H_{11}BrN_2O_2S$ (%): C, 55.49; H, 2.70; N, 6.81; S, 7.80; found: C, 55.60; H, 2.74; N, 6.83; S, 7.86.

1.4.6 Synthesis of compound **QPO-Br**



A mixture of **6** (3.0 g, 7.32 mmol) and trifluoromethanesulfonic acid (15 mL) in 100 mL single neck round bottom flask was stirred for 12 hours at 80 °C under an air atmosphere. After cooling to room temperature, the mixture was poured into 150 mL ice water and filtered to get crude product. The crude product was purified by column chromatography on silica gel using PE/ DCM (1/1, v/v) as eluent to afford **QPO-Br** as yellow powder (0.9 g, 30%). ^{1}H NMR (400 MHz, DMSO-d_6) δ 8.47 (ddd, J = 11.2, 7.7, 1.5 Hz, 2H), 8.36 (dd, J = 7.8, 1.5 Hz, 1H), 8.19 (dd, J = 7.8, 1.5 Hz, 1H), 8.12 (dd, J = 7.8, 1.5 Hz, 1H), 7.80 (t, J = 7.7 Hz, 1H), 7.67 (td, J = 8.5, 8.0, 1.6 Hz, 1H), 7.64 – 7.54 (m, 2H), 7.27 (d, J = 7.9 Hz, 1H). ^{13}C NMR (101 MHz, DMSO-d_6) δ 177.6, 140.9, 140.6, 140.3, 138.9, 133.4, 131.7, 130.2, 129.1, 128.5, 128.2, 128.0, 127.0, 126.6, 125.6, 124.9, 123.9, 122.9, 116.3. MALDI-MS (m/z) of C19H10BrNO3S for $[M+H]^+$: calcd. 410.96; found, 413.13. Anal. calcd for $C_{19}H_{10}BrNO_3S$ (%): C, 55.36; H, 2.45; N, 3.40; S, 7.78; found: C, 55.40; H, 2.51; N, 3.42; S, 7.72.

1.4.7 Synthesis of compound **QPO-PhCz**



A mixture of **QPO-Br** (0.9 g, 2.19 mmol), 4-(9*H*-carbazol-9-yl) phenylboronic acid (0.8 g, 2.63 mmol), aqueous K_2CO_3 (2.0 M, 5 mL) and $Pd(PPh_3)_4$ (0.1 g, 0.11 mmol) in 100 mL tetrahydrofuran (THF) was stirred for 24 hours at 65 °C under a nitrogen

atmosphere. After cooled to room temperature, the mixture was extracted with dichloromethane solution (4×30 mL), and the combined organic layer with dichloromethane solution was dried over $MgSO_4$. We used rotary evaporation to remove off the solvent and used silica gel column to pass the residue, which using PE/ DCM (v/v, 1:1) as an eluent to obtain **QPO-PhCz** as yellow solid (0.8 g, 61%). ^{1}H NMR (400 MHz, $CDCl_3$) δ 8.73 – 8.63 (m, 1H), 8.62 – 8.54 (m, 1H), 8.43 (d, *J* = 7.5 Hz, 1H), 8.13 (d, *J* = 7.7 Hz, 2H), 7.93 (d, *J* = 6.0 Hz, 2H), 7.77 – 7.60 (m, 4H), 7.43 (t, *J* = 6.8 Hz, 4H), 7.30 (d, *J* = 7.5 Hz, 2H), 7.24 – 7.11 (m, 4H), 7.10 – 7.02 (m, 1H). ^{13}C NMR (101 MHz, $CDCl_3$) δ 178.5, 140.6, 137.7, 137.3, 137.1, 134.4, 131.9, 131.8, 128.8, 127.4, 126.5, 125.9, 125.5, 124.8, 124.2, 123.4, 121.9, 120.4, 120.1, 109.7. MALDI-MS (m/z) of C37H22N2O3S for $[M+H]^+$: calcd. 574.14; found, 574.09. Anal. calcd for $C_{37}H_{22}N_2O_3S$ (%): C, 77.33; H, 3.86; N, 4.87; S, 5.58; found: C, 77.26; H, 3.82; N, 4.95; S, 5.61.

1.5 Density functional theory

The structural optimization of **QPO** and **QPO-PhCz** were conducted with the geometries obtained from the X-ray crystallographic analyses. The ground state moments of **QPO** and **QPO-PhCz** were obtained using density functional theory (DFT) method by adopting B3LYP/6-31g(d) level of theory.

Cartesian coordinates of **QPO** in ground state:

S	-2.43087400	0.55504700	0.76250300
O	-3.72384800	1.06250200	0.39908500

O	-2.17333900	0.31417800	2.15803500
O	3.41235800	2.00352100	-1.11385100
N	0.30911100	-0.35570700	0.05034300
C	-2.07413700	-0.90571300	-0.12138200
C	-1.17049900	1.58510800	0.12331700
C	-3.11024400	-1.72728500	-0.56154200
H	-4.01365800	-1.46145300	-0.43450800
C	-0.73270900	-1.24782700	-0.32589800
C	2.72213000	-0.00379600	-0.06376400
C	-1.41028300	2.93184500	-0.08764400
H	-2.28600400	3.28345900	0.02547700
C	0.09886800	1.02041100	-0.06392600
C	-0.45736600	-2.44580000	-0.99634300
H	0.44200900	-2.69058800	-1.17892400
C	-0.36819300	3.76937200	-0.46480200
H	-0.52557700	4.69293800	-0.62188100
C	1.85434200	-2.06494300	0.86142200
H	1.11998700	-2.62282900	1.08892500
C	-1.49155000	-3.27442000	-1.39289300
H	-1.28880100	-4.09840800	-1.81969800
C	2.51981700	1.34727400	-0.59923800
C	-2.82454800	-2.92675300	-1.18055600

H	-3.52480500	-3.50553300	-1.45769100
C	4.02167800	-0.46371700	0.18967400
H	4.76393600	0.07886300	-0.04810100
C	1.15703900	1.88227000	-0.41739300
C	1.62941900	-0.81875200	0.26484800
C	4.23952000	-1.68720300	0.77815900
H	5.12398200	-1.98794600	0.95061200
C	0.90080400	3.24190200	-0.60923600
H	1.61751800	3.81917500	-0.84494000
C	3.14438600	-2.48144700	1.11853000
H	3.28942400	-3.32324900	1.53413800

Cartesian coordinates of **QPO-PhCz** in ground state:

S	1.92428300	-2.52130300	-0.48825500
O	1.36334500	-2.04715200	-1.71936100
O	1.87828200	-3.92960300	-0.21526400
O	6.41540300	1.84889700	0.01080800
N	2.65871500	0.25509500	0.12632000
N	-3.63487300	0.38639300	-0.34253600
C	1.66190000	-0.28961500	0.99744500
C	3.75351800	-0.56777600	-0.17296900
C	2.79056800	1.66189700	-0.04911300

C	3.57143400	-1.94088200	-0.35319700
C	-5.33273100	-1.13587900	-0.22170400
C	5.06000800	-0.06037700	-0.23219400
C	1.24215800	-1.61569500	0.83042200
C	1.13616400	0.43925300	2.05843600
H	1.42823800	1.32951200	2.21359100
C	-4.83014400	1.10365300	-0.26113400
C	1.66203600	2.48671300	-0.21222400
C	-0.71883200	2.48772100	0.51769300
H	-0.50980600	3.21357700	1.09324400
C	-0.07719000	0.94715900	-1.20489200
H	0.58245400	0.58601900	-1.78580400
C	0.26835400	1.96647200	-0.31567500
C	-2.00117300	1.96626400	0.51936000
H	-2.65354400	2.30442400	1.12127100
C	-1.36880400	0.45800400	-1.24608700
H	-1.60367200	-0.21024900	-1.87917700
C	-3.93140200	-0.98184500	-0.30616100
C	4.08093100	2.22654200	-0.09631100
C	-2.32883500	0.94574100	-0.36061400
C	-5.89728700	0.19375900	-0.18412100
C	6.12738800	-0.94142400	-0.38593100

H	7.01025700	-0.59362000	-0.43344400
C	-5.87865000	-2.41375600	-0.17370100
H	-6.82059900	-2.53454400	-0.14669900
C	0.19029400	-0.13071400	2.88567100
H	-0.18237500	0.38417800	3.59149900
C	0.31487200	-2.19440900	1.69062200
H	0.05698600	-3.10162100	1.57809600
C	-3.07363000	-2.07665600	-0.27657400
H	-2.13111200	-1.96569500	-0.30614900
C	5.28520800	1.38439500	-0.07980600
C	-7.21035700	0.66966300	-0.10960100
H	-7.94333300	0.06751900	-0.05504800
C	4.63997700	-2.80483200	-0.47206000
H	4.48929400	-3.73924600	-0.55514500
C	1.85977300	3.85910500	-0.29492800
H	1.10324300	4.42913800	-0.36180900
C	-7.41823900	2.03406100	-0.11876500
H	-8.30339400	2.37237700	-0.05286300
C	5.94089000	-2.30676800	-0.47084800
H	6.68451000	-2.89461600	-0.52793900
C	-3.64547100	-3.32983100	-0.20197800
H	-3.08256500	-4.09474300	-0.17374000

C	-5.03675200	-3.50246800	-0.16590400
H	-5.40171400	-4.37876400	-0.13574700
C	-0.22467400	-1.43756700	2.70698200
H	-0.87988100	-1.81299300	3.28335100
C	-5.04375300	2.47871600	-0.29550900
H	-4.31932900	3.08871100	-0.36606600
C	-6.35179700	2.92218100	-0.22039500
H	-6.52656500	3.85604600	-0.24093200
C	4.22741900	3.60925100	-0.20743100
H	5.09852900	3.98829300	-0.23145400
C	3.13246100	4.42511900	-0.28149700
H	3.23891800	5.36855100	-0.32472800

2 Supplemental Figures

2.1 Structural properties

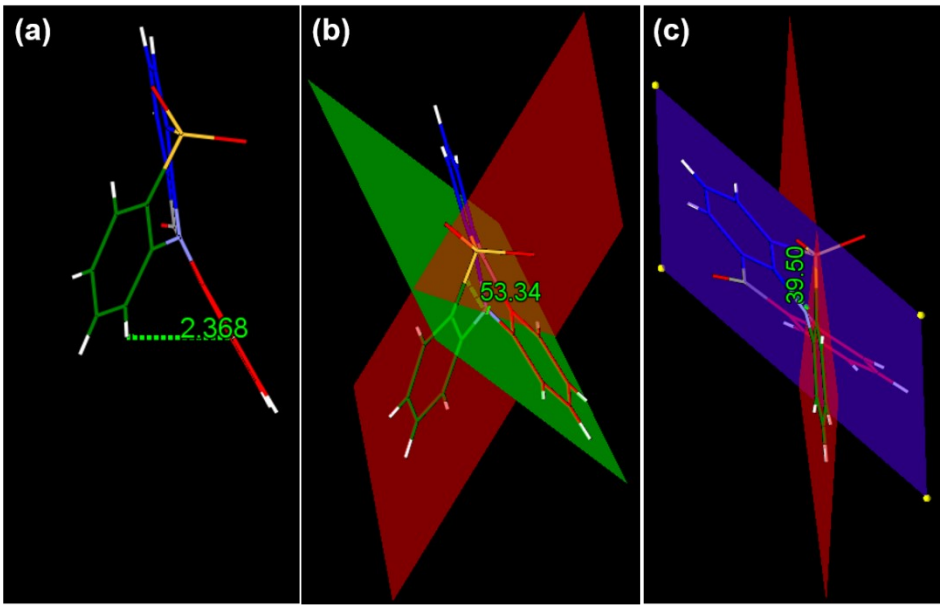


Figure S1. The details structure of **QPO**.

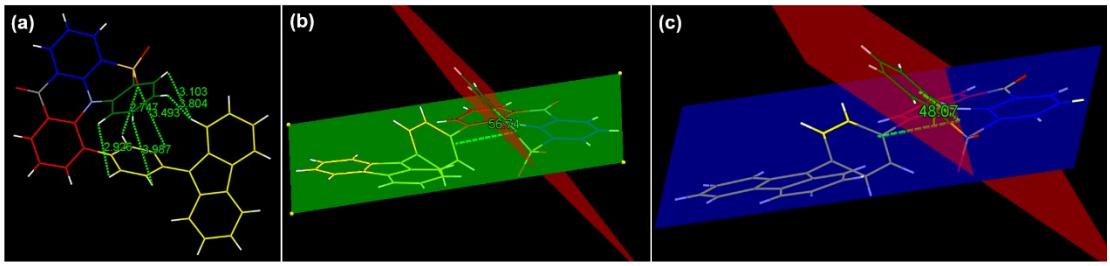


Figure S2. The details structure of **QPO-PhCz**.

2.2 Photophysical properties

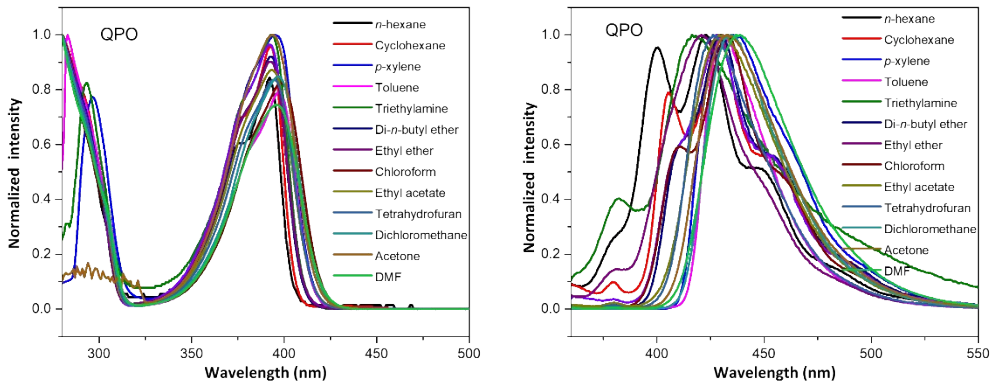


Figure S3. Solvent effect on the ultraviolet–visible absorption spectra and photoluminescence spectra of **QPO**.

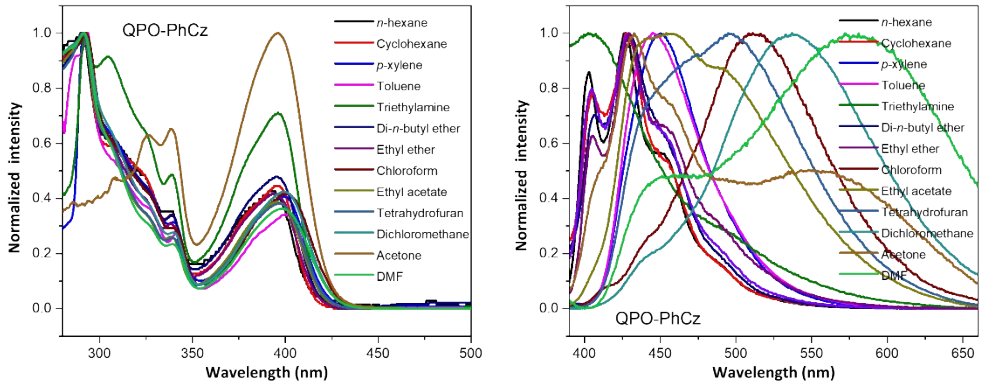


Figure S4. Solvent effect on the ultraviolet–visible absorption spectra and photoluminescence spectra of **QPO-PhCz**.

2.3 Theoretical calculation

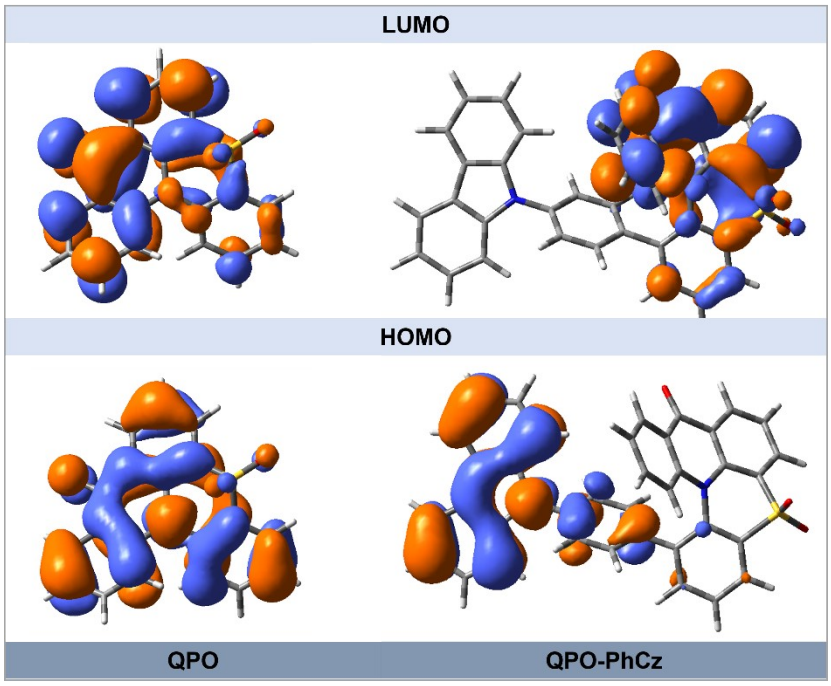


Figure S5. HOMO and LUMO orbital distributions based on DFT at the B3LYP functional and 6-31G(d) basis set.

2.4 Chiroptical properties

Operator:Administrator Timebase:HPLC Sequence:20180108

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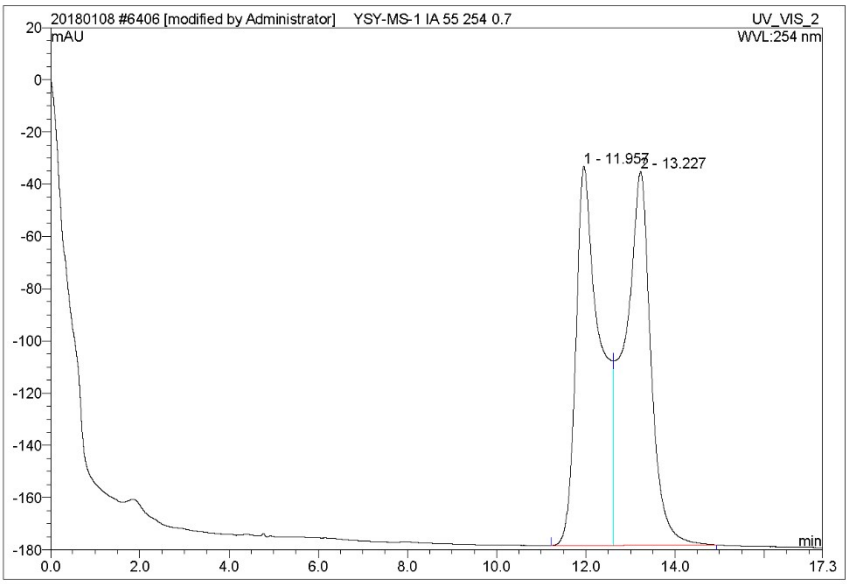
2019-7-10 2:45 下午

6406 YSY-MS-1 IA 55 254 0.7

Sample Name:	**YSY-MS-1 IA 55 254 0.7**	*Injection Volume:*	**2.0**
Vial Number:	**RB3**	*Channel:*	**UV_VIS_2**
Sample Type:	**unknown**	*Wavelength:*	**254.0**
Control Program:	**test-dad4**	*Bandwidth:*	**4**
Quantif. Method:	**20170608**	*Dilution Factor:*	**1.0000**
Recording Time:	**2019-7-10 14:07**	*Sample Weight:*	**1.0000**
Run Time (min):	**17.30**	*Sample Amount:*	**1.0000**



No.	Ret.Time min	Peak Name	Height mAU	Area mAU*min	Rel.Area %	Amount	Type
1	11.96	n.a.	145.169	91.435	48.43	n.a.	BM
2	13.23	n.a.	143.109	97.360	51.57	n.a.	MB
Total:			288.278	188.795	100.00	0.000	

default/Integration

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Figure S6. HPLC profile of **QPO**.

Operator:Administrator Timebase:HPLC Sequence:20180108

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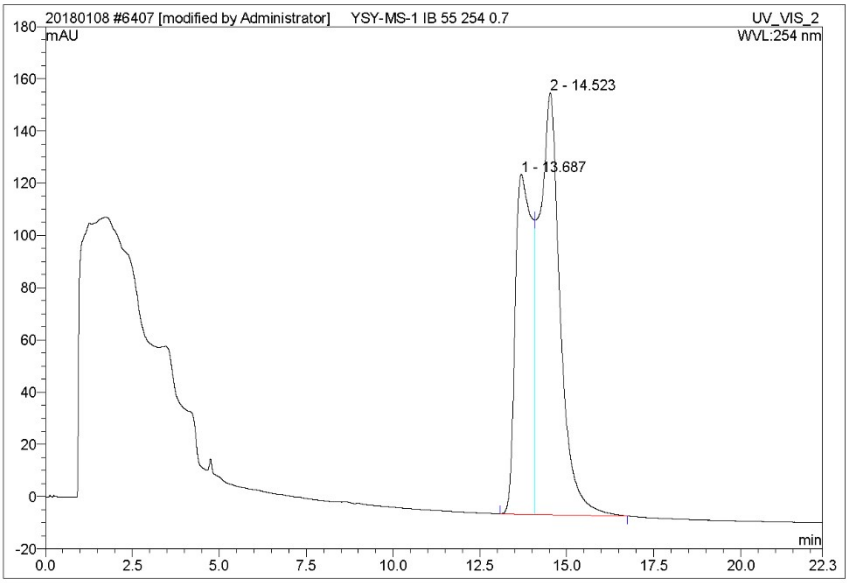
2019-7-10 2:53 下午

6407 YSY-MS-1 IB 55 254 0.7

Sample Name:	**YSY-MS-1 IB 55 254 0.7**	*Injection Volume:*	**2.0**
Vial Number:	**RB3**	*Channel:*	**UV_VIS_2**
Sample Type:	**unknown**	*Wavelength:*	**254.0**
Control Program:	**test-dad4**	*Bandwidth:*	**4**
Quantif. Method:	**20170608**	*Dilution Factor:*	**1.0000**
Recording Time:	**2019-7-10 14:30**	*Sample Weight:*	**1.0000**
Run Time (min):	**22.35**	*Sample Amount:*	**1.0000**



No.	Ret.Time min	Peak Name	Height mAU	Area mAU*min	Rel.Area %	Amount	Type
1	13.69	n.a.	129.969	73.607	39.43	n.a.	BM
2	14.52	n.a.	161.539	113.055	60.57	n.a.	MB
Total:			291.507	186.662	100.00	0.000	

default/Integration

Chromeleon (c) Dionex 1996-2006
Version 6.80 SR14 Build 4527 (238909)

Figure S7. HPLC profile of **QPO**.

Operator:Administrator Timebase:HPLC Sequence:20180108

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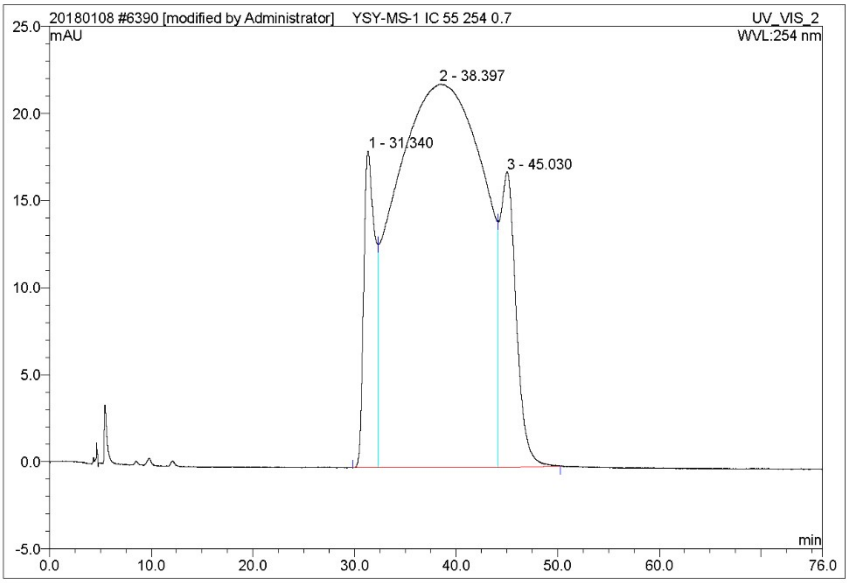
2019-7-10 2:34 下午

6390 YSY-MS-1 IC 55 254 0.7

Sample Name:	**YSY-MS-1 IC 55 254 0.7**	*Injection Volume:*	**3.0**
Vial Number:	**RB5**	*Channel:*	**UV_VIS_2**
Sample Type:	**unknown**	*Wavelength:*	**254.0**
Control Program:	**test-dad4**	*Bandwidth:*	**4**
Quantif. Method:	**20170608**	*Dilution Factor:*	**1.0000**
Recording Time:	**2019-7-9 15:30**	*Sample Weight:*	**1.0000**
Run Time (min):	**76.05**	*Sample Amount:*	**1.0000**



No.	Ret.Time min	Peak Name	Height mAU	Area mAU*min	Rel.Area %	Amount	Type
1	31.34	n.a.	18.218	23.697	8.56	n.a.	BM *
2	38.40	n.a.	22.050	221.236	79.96	n.a.	M *
3	45.03	n.a.	16.987	31.759	11.48	n.a.	MB*
Total:			57.255	276.691	100.00	0.000	

default/Integration

Chromeleon (c) Dionex 1996-2006
Version 6.80 SR14 Build 4527 (238909)

Figure S8. HPLC profile of **QPO**.

Operator:Administrator Timebase:HPLC Sequence:20180108

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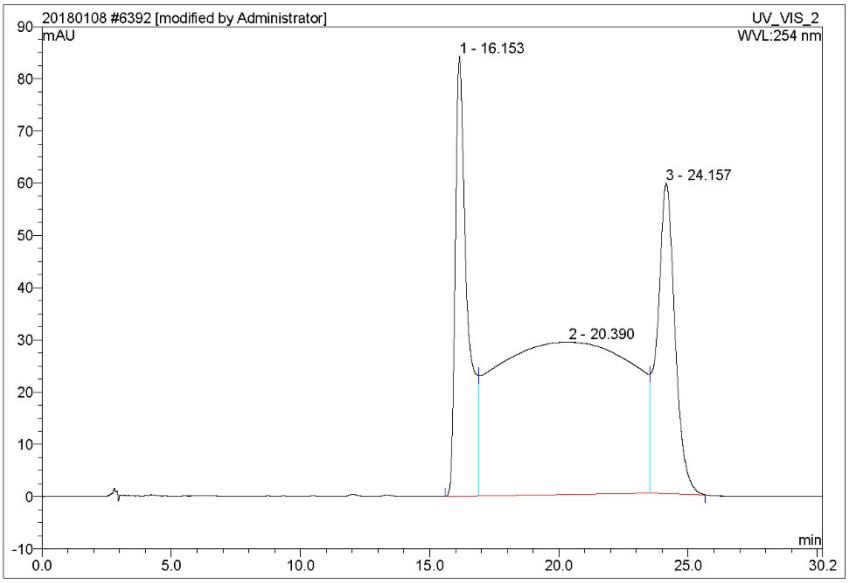
6392 YSY-MS-1 ID3 55 254 0.7

Sample Name:	**YSY-MS-1 ID3 55 254 0.7**	*Injection Volume:*	**3.0**
Vial Number:	**RB5**	*Channel:*	**UV_VIS_2**
Sample Type:	**unknown**	*Wavelength:*	**254.0**
Control Program:	**test-dad4**	*Bandwidth:*	**4**
Quantif. Method:	**20170608**	*Dilution Factor:*	**1.0000**
Recording Time:	**2019-7-9 17:27**	*Sample Weight:*	**1.0000**
Run Time (min):	**30.20**	*Sample Amount:*	**1.0000**



No.	Ret.Time min	Peak Name	Height mAU	Area mAU*min	Rel.Area %	Amount	Type
1	16.15	n.a.	84.192	45.533	16.77	n.a.	BM *
2	20.39	n.a.	29.193	178.611	65.79	n.a.	M *
3	24.16	n.a.	59.380	47.342	17.44	n.a.	MB*
Total:			172.766	271.486	100.00	0.000	

default/Integration

Chromeleon (c) Dionex 1996-2006
Version 6.80 SR14 Build 4527 (238909)

Figure S9. HPLC profile of **QPO**.

Operator:Administrator Timebase:HPLC Sequence:20180108

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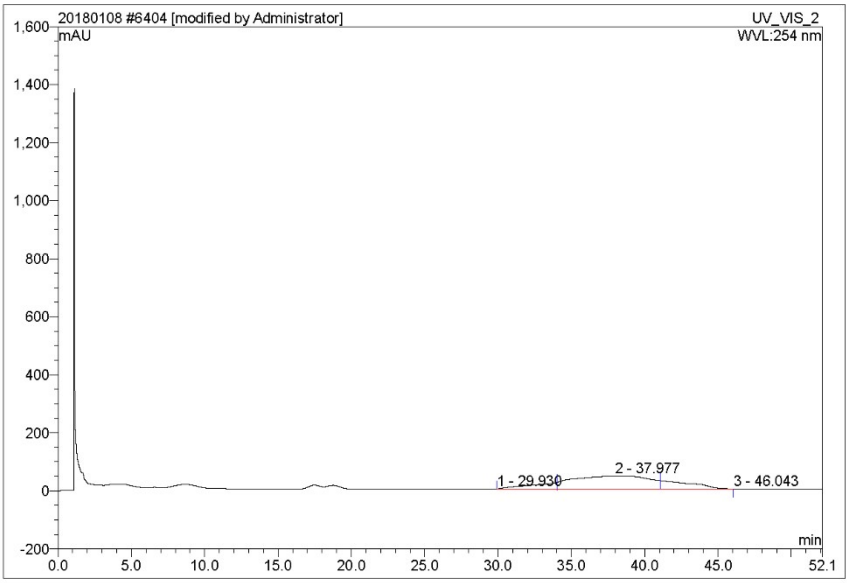
6404 YSY-MS-1 IE3 55 254 0.7

Sample Name:	**YSY-MS-1 IE3 55 254 0.7**	*Injection Volume:*	**2.0**
Vial Number:	**RB3**	*Channel:*	**UV_VIS_2**
Sample Type:	**unknown**	*Wavelength:*	**254.0**
Control Program:	**test-dad4**	*Bandwidth:*	**4**
Quantif. Method:	**20170608**	*Dilution Factor:*	**1.0000**
Recording Time:	**2019-7-10 12:06**	*Sample Weight:*	**1.0000**
Run Time (min):	**52.12**	*Sample Amount:*	**1.0000**



No.	Ret.Time min	Peak Name	Height mAU	Area mAU*min	Rel.Area %	Amount	Type
1	29.93	n.a.	0.010	45.901	12.07	n.a.	BM *
2	37.98	n.a.	43.273	265.028	69.71	n.a.	M *
3	46.04	n.a.	0.004	69.277	18.22	n.a.	MB*
Total:			43.287	380.206	100.00	0.000	

default/Integration

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Figure S10. HPLC profile of **QPO**.

Operator:Administrator Timebase:HPLC Sequence:20180108

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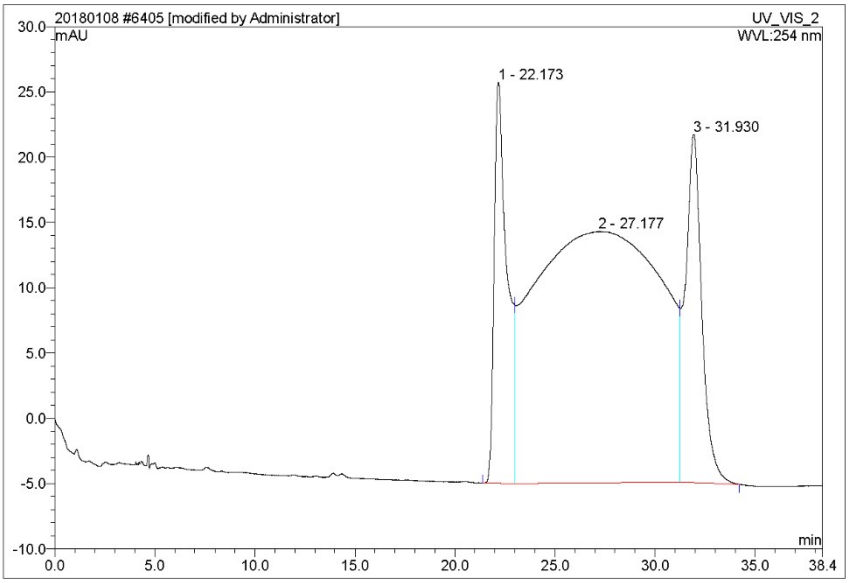
6405 YSY-MS-1 IF3 55 254 0.7

Sample Name:	**YSY-MS-1 IF3 55 254 0.7**	*Injection Volume:*	**2.0**
Vial Number:	**RB3**	*Channel:*	**UV_VIS_2**
Sample Type:	**unknown**	*Wavelength:*	**254.0**
Control Program:	**test-dad4**	*Bandwidth:*	**4**
Quantif. Method:	**20170608**	*Dilution Factor:*	**1.0000**
Recording Time:	**2019-7-10 13:17**	*Sample Weight:*	**1.0000**
Run Time (min):	**38.36**	*Sample Amount:*	**1.0000**



No.	Ret.Time min	Peak Name	Height mAU	Area mAU*min	Rel.Area %	Amount	Type
1	22.17	n.a.	30.711	22.934	12.08	n.a.	BM *
2	27.18	n.a.	19.230	141.342	74.43	n.a.	M *
3	31.93	n.a.	26.651	25.636	13.50	n.a.	MB*
Total:			76.591	189.911	100.00	0.000	

default/Integration

Chromeleon (c) Dionex 1996-2006
Version 6.80 SR14 Build 4527 (238909)

Figure S11. HPLC profile of **QPO**.

Operator:Administrator Timebase:HPLC Sequence:20180108

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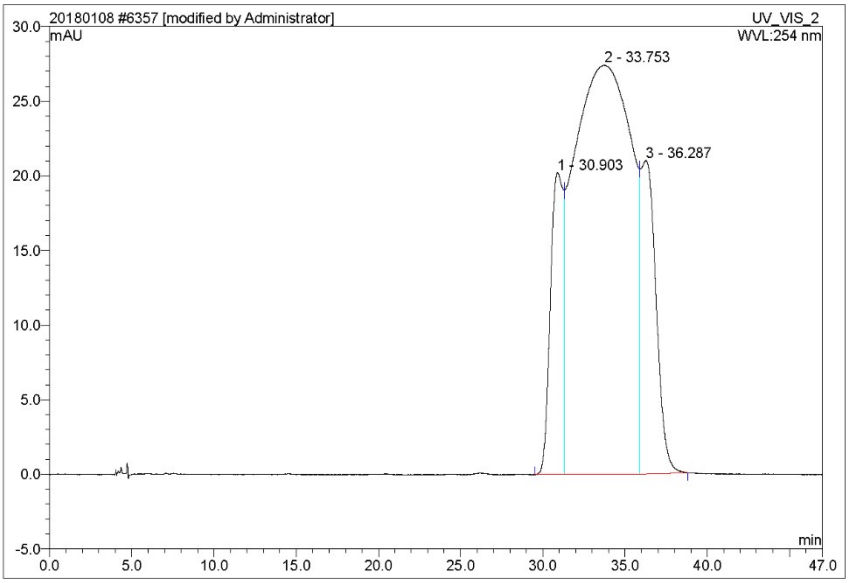
2019-7-10 2:33 下午

6357 YSY-MS-1 IG 55 254 0.7

Sample Name:	**YSY-MS-1 IG 55 254 0.7**	*Injection Volume:*	**2.0**
Vial Number:	**RA4**	*Channel:*	**UV_VIS_2**
Sample Type:	**unknown**	*Wavelength:*	**254.0**
Control Program:	**test-dad6**	*Bandwidth:*	**4**
Quantif. Method:	**20170608**	*Dilution Factor:*	**1.0000**
Recording Time:	**2019-7-5 12:23**	*Sample Weight:*	**1.0000**
Run Time (min):	**47.00**	*Sample Amount:*	**1.0000**



No.	Ret.Time min	Peak Name	Height mAU	Area mAU*min	Rel.Area %	Amount	Type
1	30.90	n.a.	20.212	18.376	12.04	n.a.	BM *
2	33.75	n.a.	27.405	110.917	72.67	n.a.	M *
3	36.29	n.a.	21.004	23.328	15.29	n.a.	MB*
Total:			68.621	152.621	100.00	0.000	

default/Integration

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Version 6.80 SR14 Build 4527 (238909)

Figure S12. HPLC profile of **QPO**.

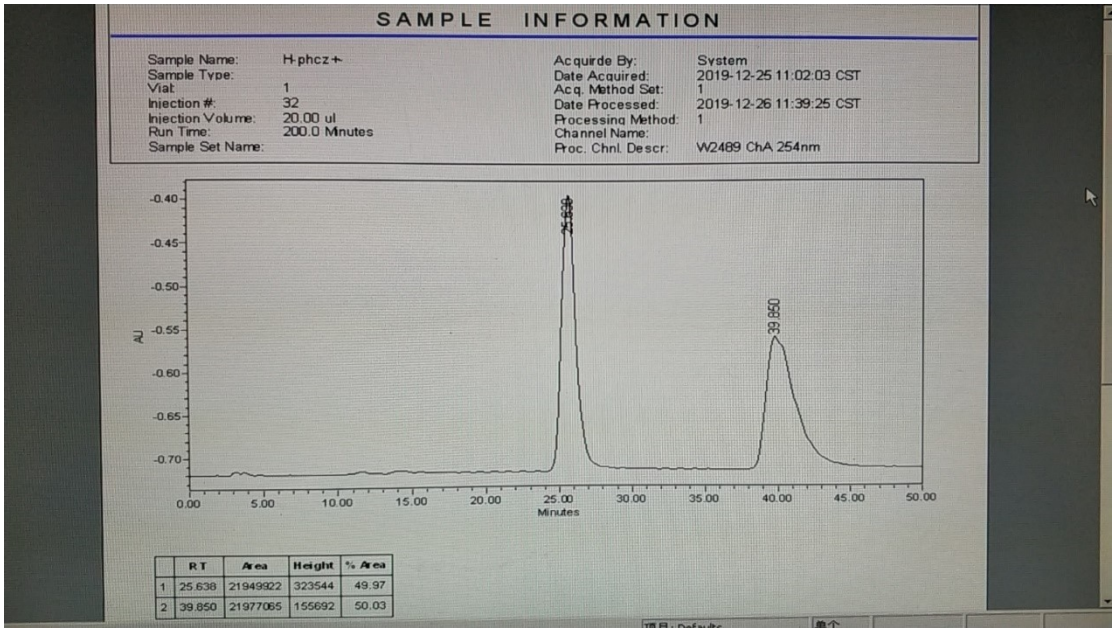


Figure S13. HPLC profile of **QPO-PhCz**.

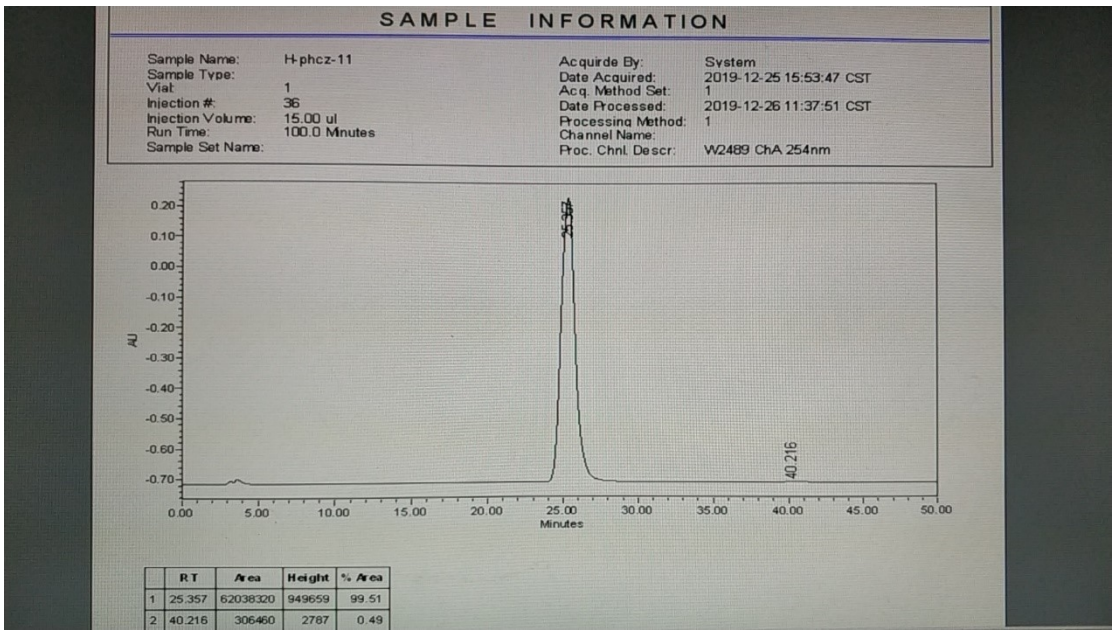


Figure S14. HPLC profile of **(M)-QPO-PhCz**.

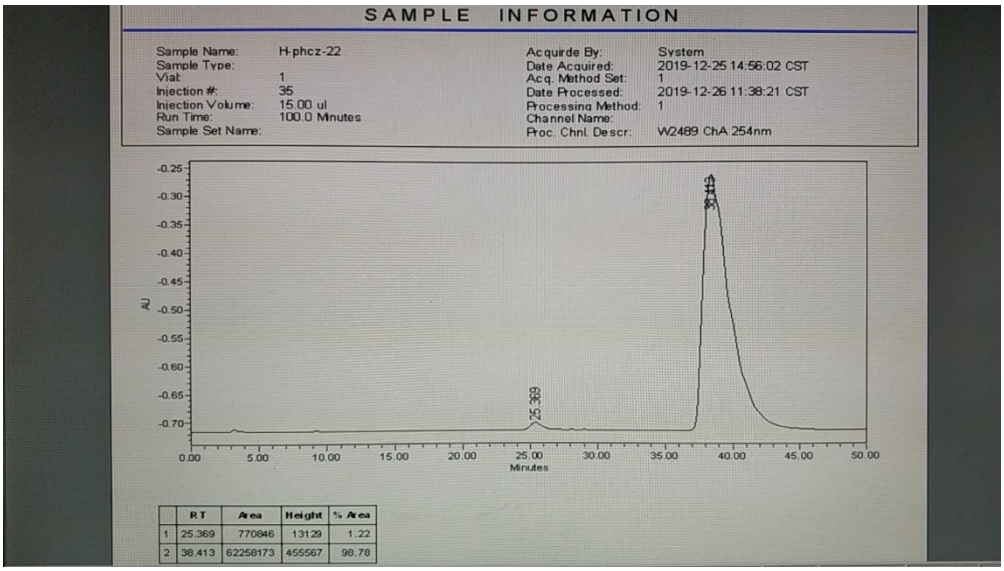


Figure S15. HPLC profile of **(P)-QPO-PhCz**.

2.5 Thermal properties

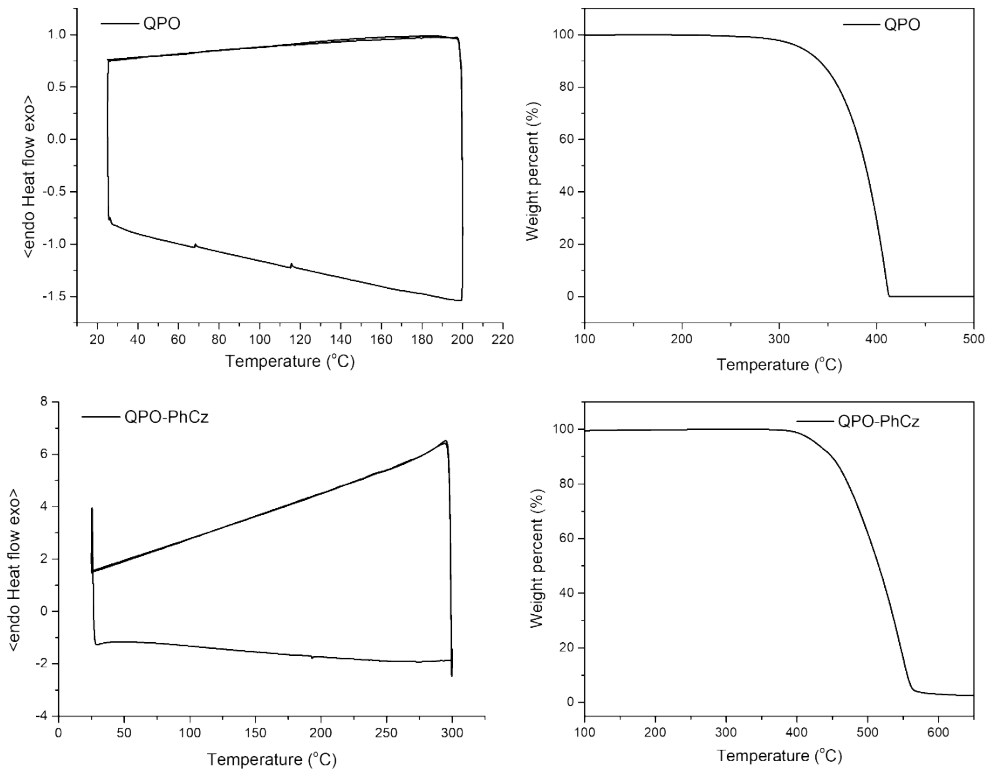


Figure S16. TGA/DSC curves of **QPO** and **QPO-PhCz**.

2.6 Electrochemical properties

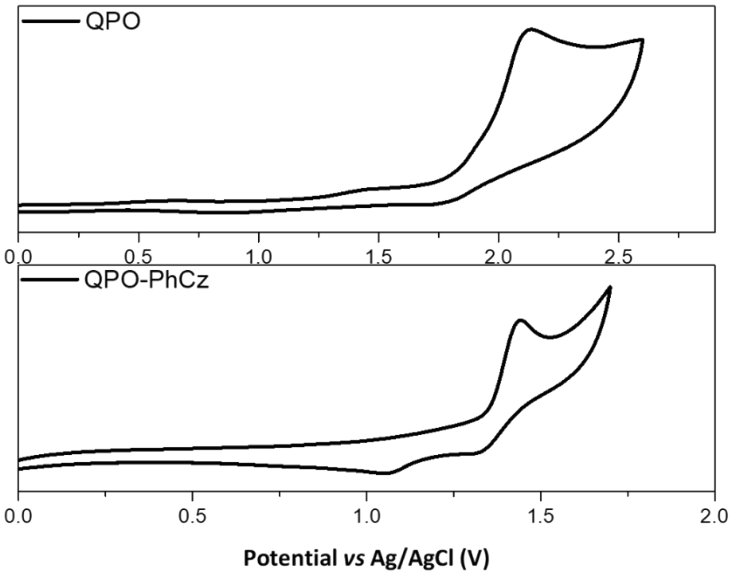


Figure S17. CV curves of **QPO** and **QPO-PhCz**.

2.7 Electroluminescence properties

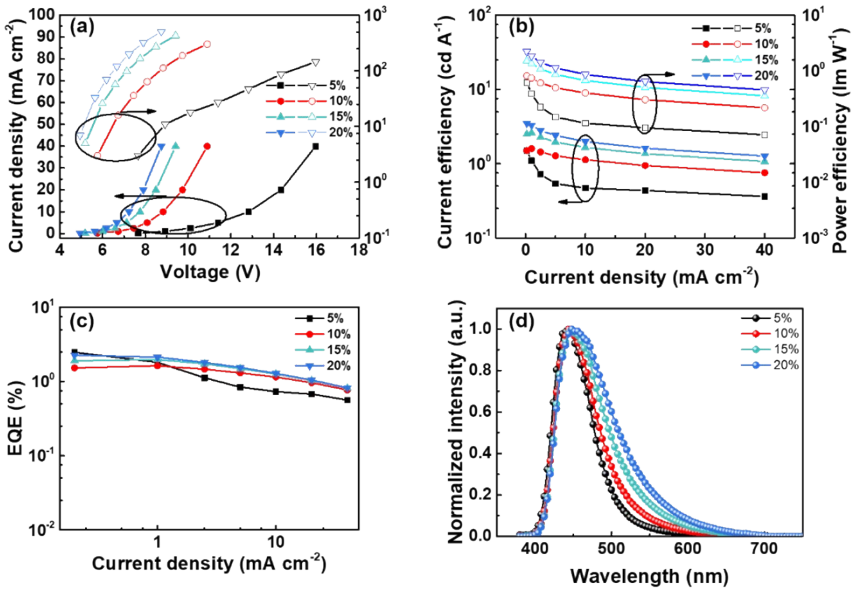


Figure S18. (a) *J*-V-L characteristics; (b) CE-J-PE characteristics; (c) EQE-J characteristics and (d) EL spectra of **QPO** doped devices.

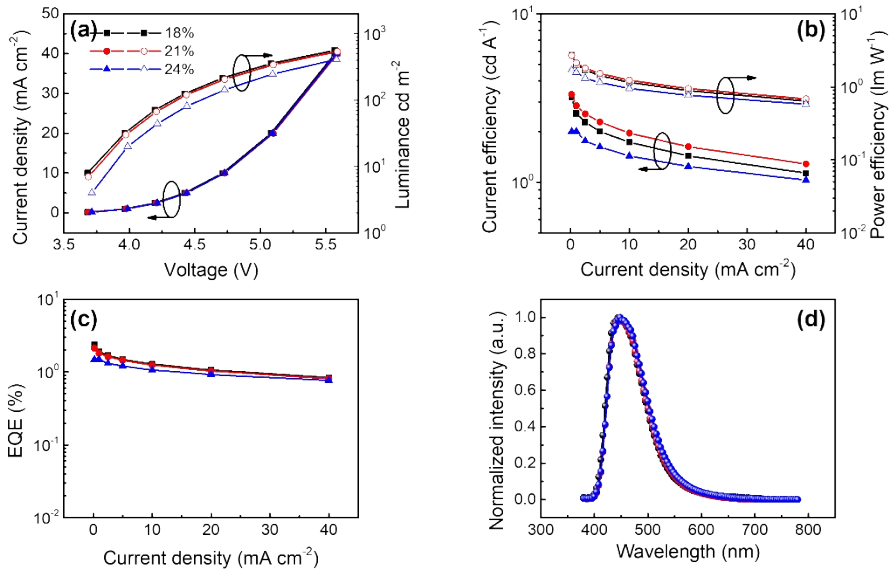


Figure S19. (a) *J*-V-L characteristics; (b) CE-J-PE characteristics; (c) EQE-J characteristics and (d) EL spectra of **QPO** doped devices.

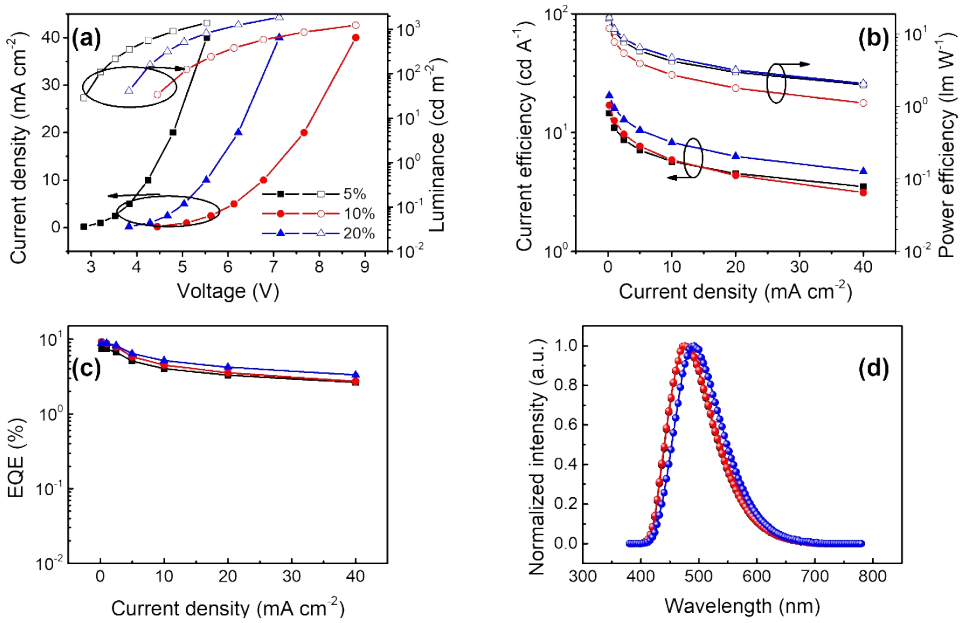


Figure S20. (a) *J*-V-L characteristics; (b) CE-J-PE characteristics; (c) EQE-J characteristics and (d) EL spectra of **QPO-PhCz** doped devices.

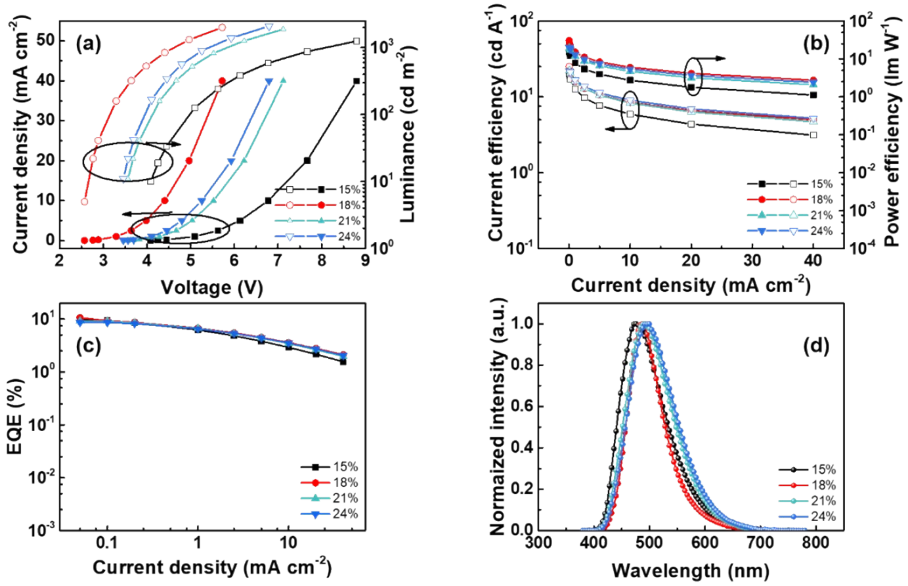


Figure S21. (a) *J*-V-L characteristics; (b) CE-J-PE characteristics; (c) EQE-J characteristics and (d) EL spectra of **QPO-PhCz** doped devices.

2.8 Circularly polarized electroluminescence properties

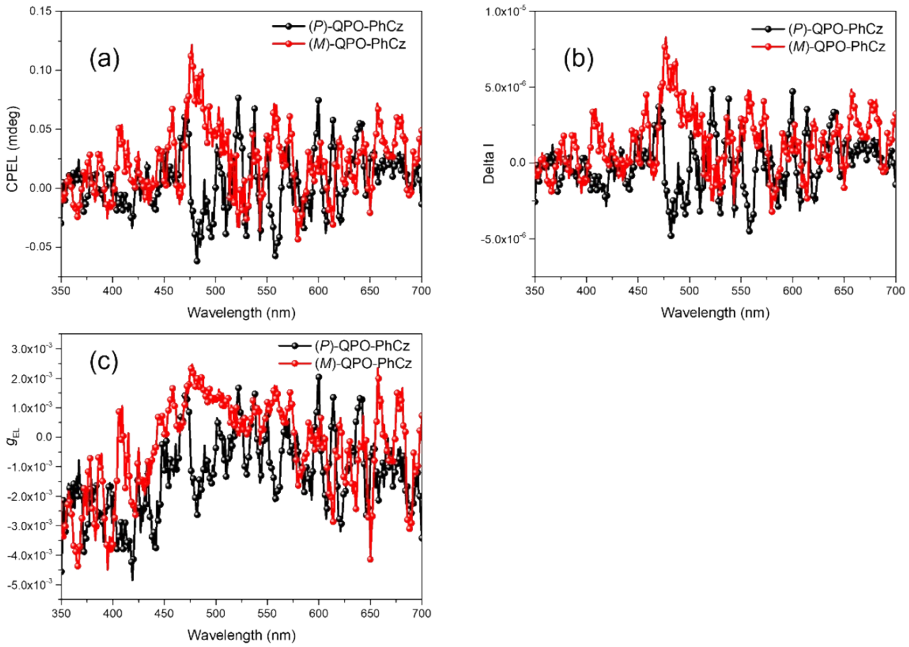


Figure S22. (a) Circularly polarized electroluminescence of **(*P*)-QPO-PhCz/ (*M*)-QPO-PhCz**; (b) CPPL spectra of **(*P*)-QPO-PhCz/ (*M*)-QPO-PhCz** based on ΔI; (c) g_{EL} curves of **(*P*)-QPO-PhCz/ (*M*)-QPO-PhCz**.

3 Supplementary Tables

3.1 Crystal data and structure refinement

Table S1 Crystal data and structure refinement for **QPO**

Empirical formula	C19H11NO3S
Formula weight	333.35
Temperature/K	100.0
Crystal system	triclinic
Space group	P-1
Unit cell dimensions	a/Å: 7.9427(4) b/Å: 8.2337(5) c/Å: 11.3541(7) α/°: 88.5360(10) β/°: 83.950(2) γ/°: 71.4370(10)
Volume/ $Å^3$	699.96(7)
Z	2
Density/g/cm^3	1.582
Absorption coefficient/mm^{-1}	0.250
F(000)	344.0
Crystal size/mm^3	0.28 × 0.15 × 0.12
Theta range for data collection/°	5.22 to 55.106
Index ranges	$-10 \leq h \leq 8$ $-10 \leq k \leq 10$ $-14 \leq l \leq 14$
Reflections collected	8610
Independent reflections	3200 [R_{int} = 0.0400, R_{sigma} = 0.0509]
Data/restraints/parameters	3200/0/217
Goodness-of-fit on F^2	1.023
Final R indices [I>2sigma(I)]	R_1 = 0.0446, wR_2 = 0.1038
R indices (all data)	R_1 = 0.0615, wR_2 = 0.1166
Largest diff. peak and hole	0.34/-0.53
Radiation	MoKα (λ = 0.71073)
CCDC number	2051469

Table S2 Crystal data and structure refinement for **QPO-PhCz**

Empirical formula	C37H22N2O3S

Formula weight	574.62
Temperature/K	173.0
Crystal system	triclinic
Space group	P-1
Unit cell dimensions	a/Å: 9.2936(6) b/Å: 10.7266(7) c/Å: 13.7992(10) α/°: 92.415(2) β/°: 98.846(2) γ/°: 104.956(2)
Volume/ $Å^3$	1308.38(15)
Z	2
Density/g/cm^3	1.459
Absorption coefficient/mm^{-1}	0.169
F(000)	596.0
Crystal size/mm^3	0.15 × 0.11 × 0.08
Theta range for data collection/°	4.604 to 52.77
Index ranges	$-11 \leq h \leq 11$ $-13 \leq k \leq 12$ $-17 \leq l \leq 17$
Reflections collected	14836
Independent reflections	5302 [R_{int} = 0.0474, R_{sigma} = 0.0604]
Data/restraints/parameters	5302/0/388
Goodness-of-fit on F^2	1.080
Final R indices [I>2sigma(I)]	R_1 = 0.0559, wR_2 = 0.1287
R indices (all data)	R_1 = 0.0873, wR_2 = 0.1478
Largest diff. peak and hole	0.35/-0.49
Radiation	MoKα (λ = 0.71073)
CCDC number	2051470

3.2 Electroluminescence characteristics

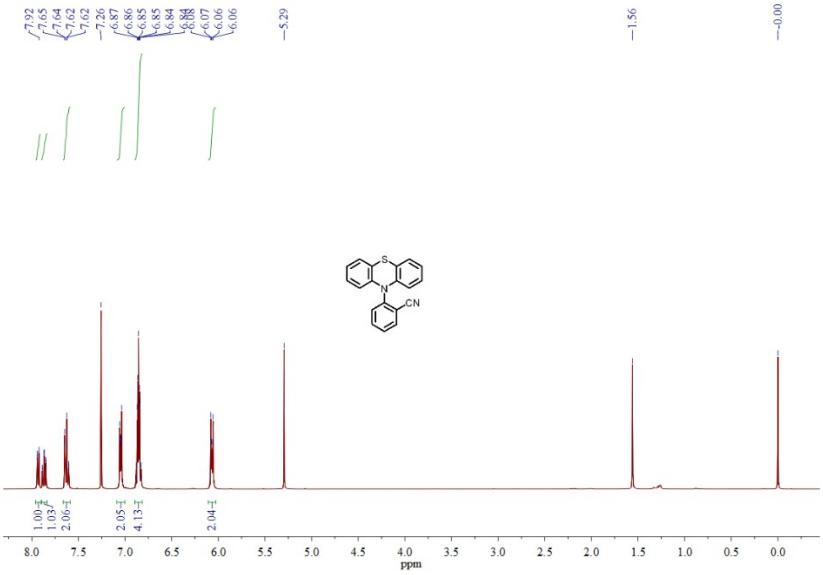
Table S3. Electroluminescence characteristics of the **QPO** and **QPO-PhCz** doped devices at different dopant concentrations.

Device	Dopant ratio	η_{CE} [a]	η_{PE} [a]	EQE [a]	Peak wavelength [b]	CIE
		(cd A^{-1})	(lm W^{-1})	(%)	(nm)	(x,y)
QPO	**5 wt%**	1.5	0.6	2.5	444	(0.16, 0.07)
	10 wt%	1.6	0.8	1.6	448	(0.16, 0.11)
	15 wt%	2.6	1.5	2.0	448	(0.16.0.15)
	18 wt%	3.2	2.7	2.4	448	(0.16, 0.11)
	20 wt%	3.5	2.2	2.3	448	(0.17,0.19)
	21 wt%	3.3	2.8	2.1	448	(0.16, 0.11)
	24 wt%	2.0	1.7	1.5	448	(0.16.0.13)
QPO-PhCz	**5 wt%**	14.5	16.0	7.4	476	(0.18, 0.28)
	10 wt%	17.0	12.0	8.8	476	(0.18, 0.29)
	15 wt%	20.0	15.4	9.4	476	(0.18, 0.28)
	18 wt%	25.0	30.5	10.6	488	(0.17, 0.34)
	20 wt%	20.5	17.2	9.2	492	(0.20.0.36)
	21 wt%	22.0	19.3	9.2	492	(0.20.0.36)
	24 wt%	22.0	20.0	8.6	500	(0.21,0.39)

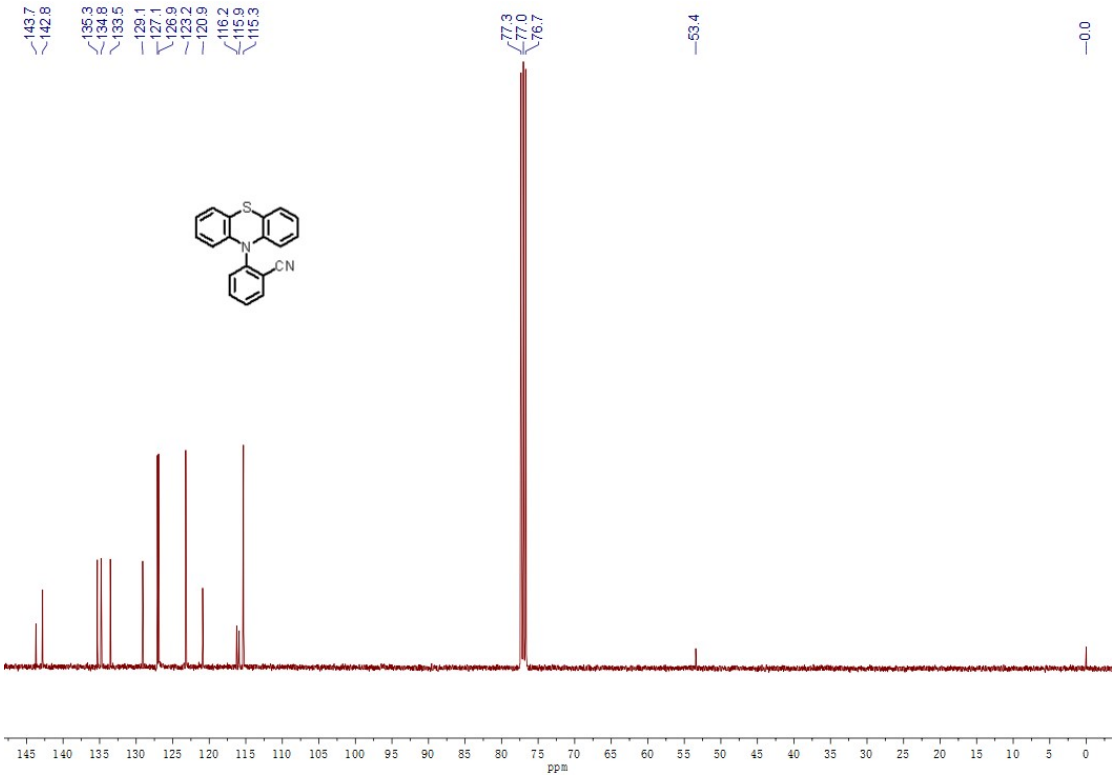
[a] Efficiencies in the order of the maxima. [b] Measured at 5 mA cm^{-2}.

4 Copy of NMR Spectra and MALDI-TOF-MS Plot

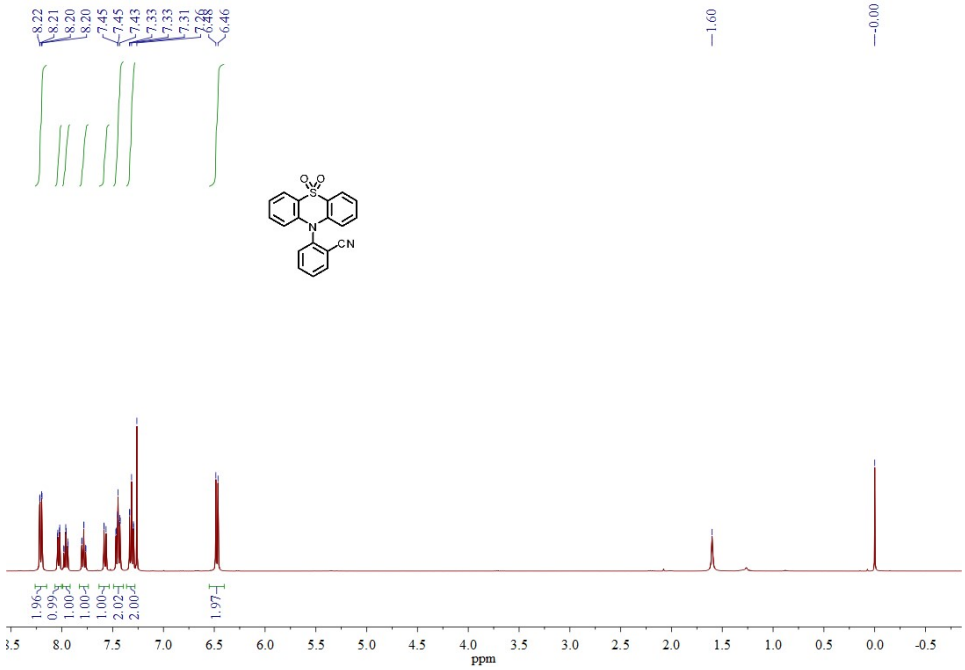
4.1 ^{1}H NMR plot of **2**, 400 MHz, $CDCl_3$



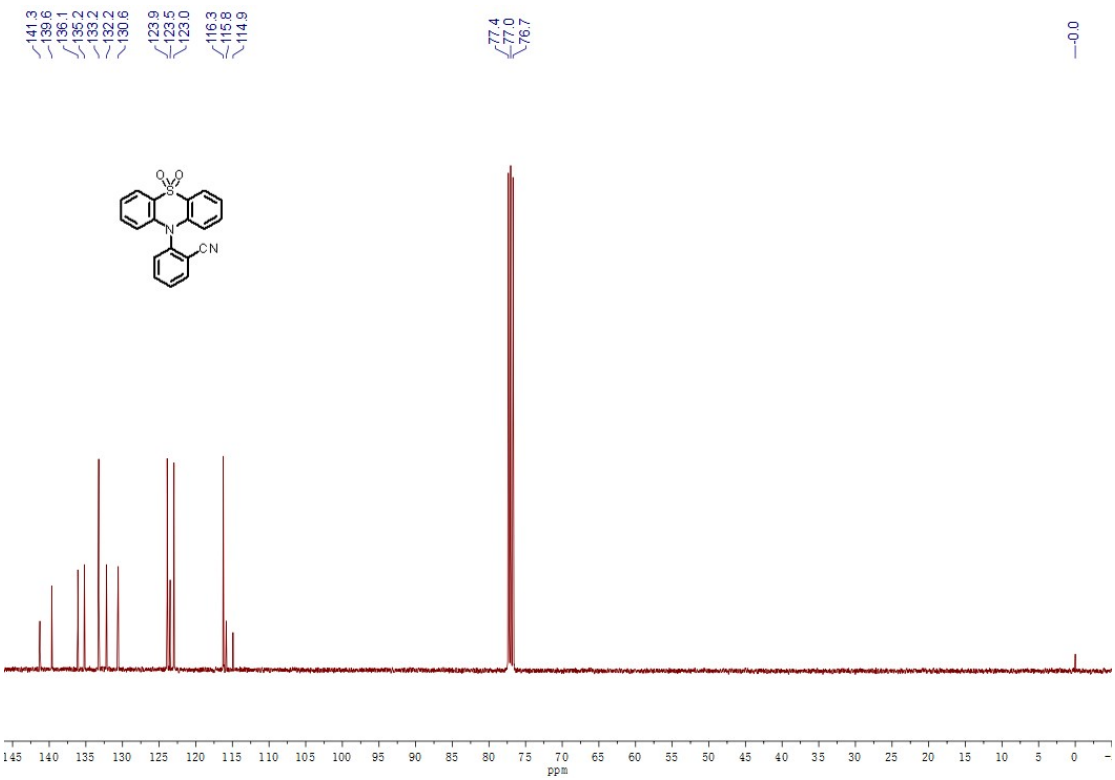
4.2 ^{13}C NMR plot of **2**, 101 MHz, $CDCl_3$



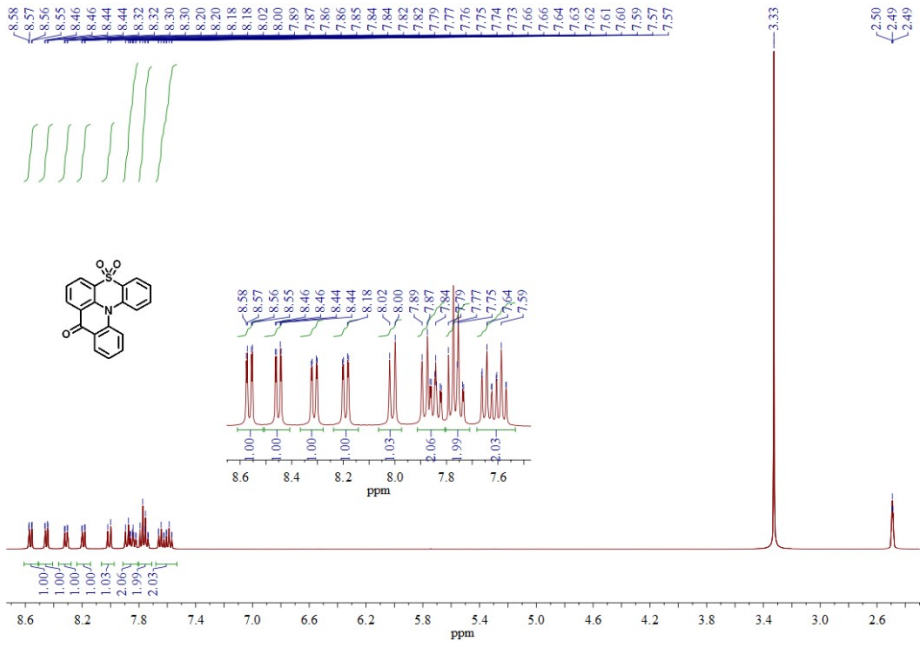
4.3 ^{1}H NMR plot of **3**, 400 MHz, $CDCl_3$



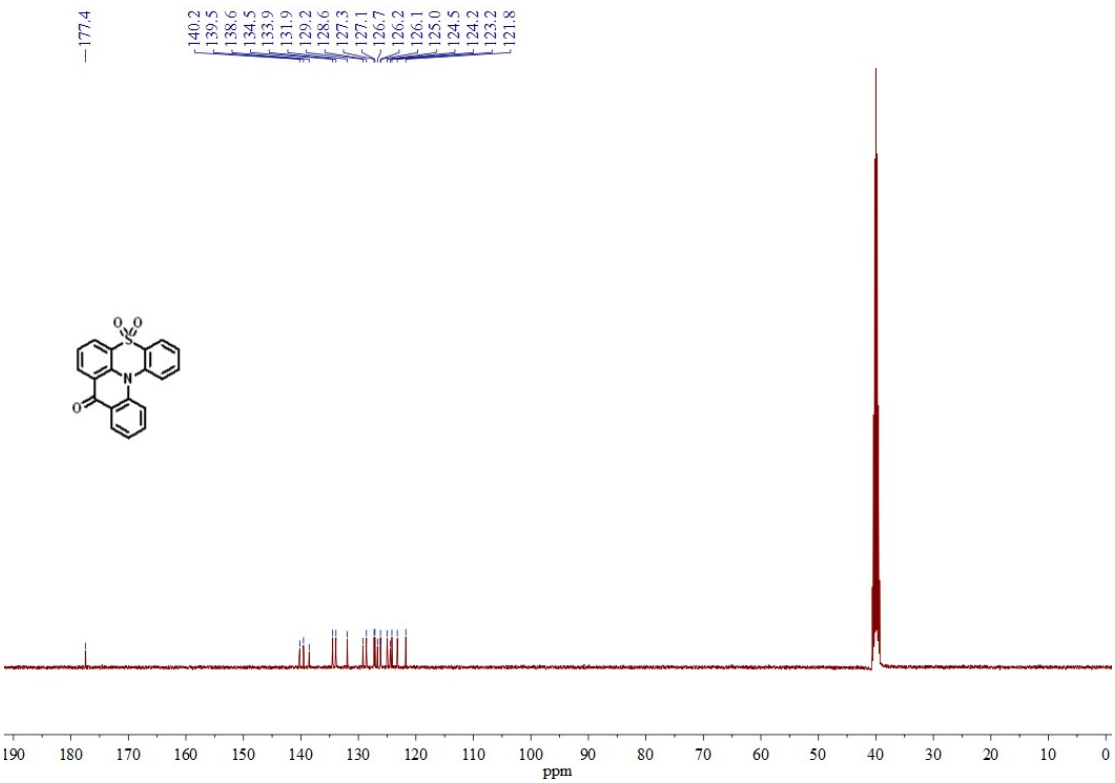
4.4 ^{13}C NMR plot of **3**, 101 MHz, $CDCl_3$



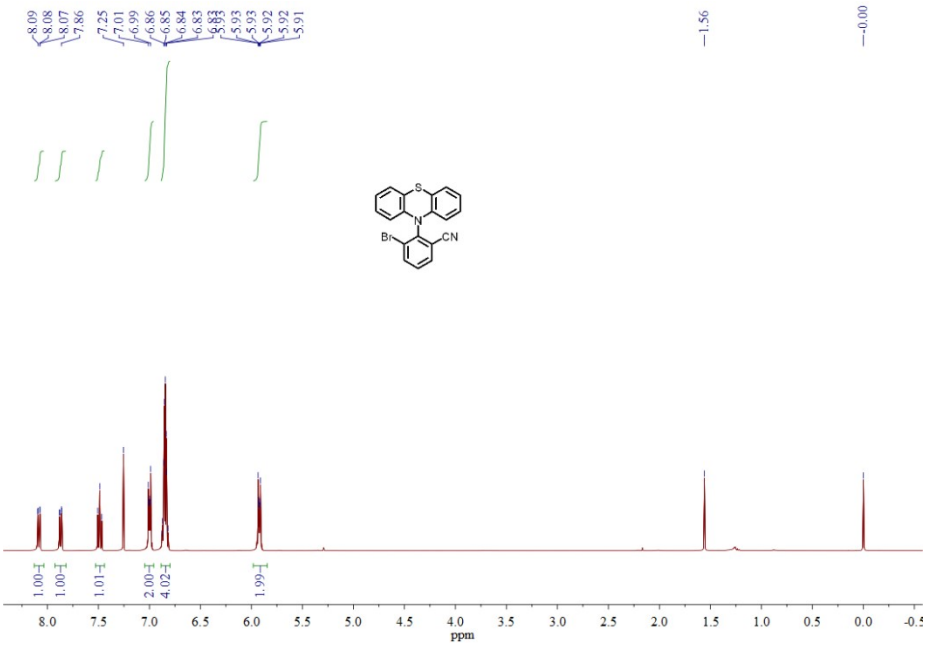
4.5 ^{1}H NMR plot of **QPO**, 400 MHz, DMSO



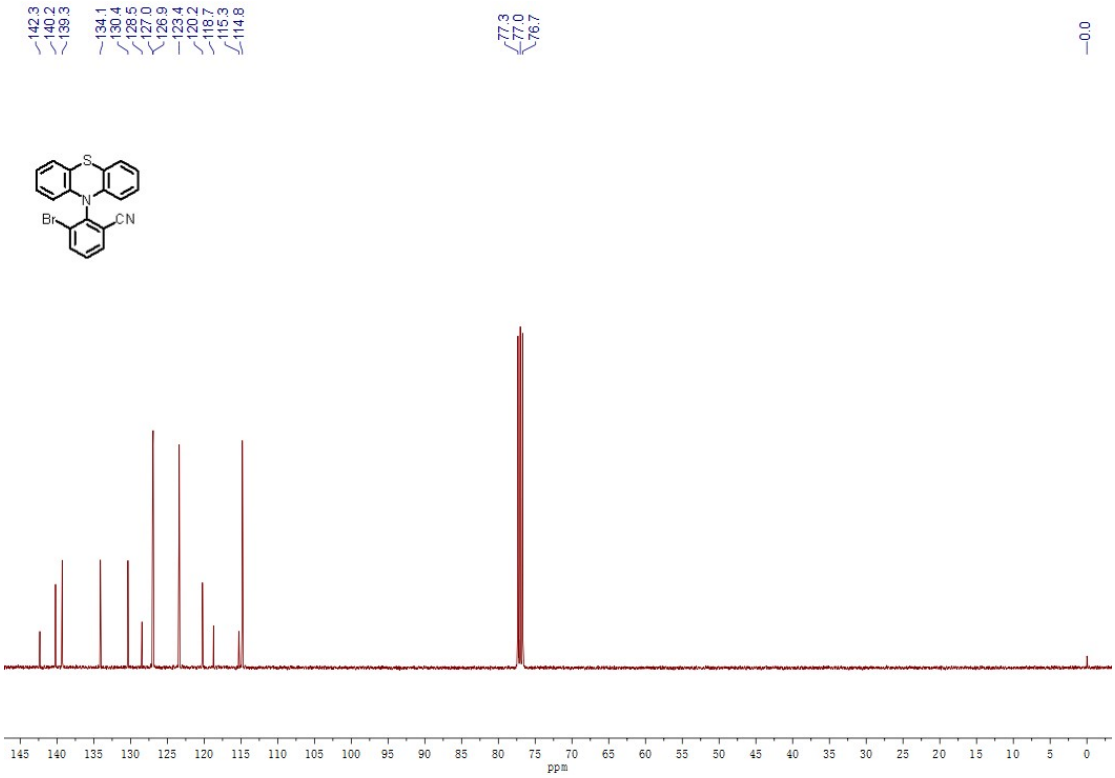
4.6 ^{13}C NMR plot of **QPO**, 101 MHz, DMSO



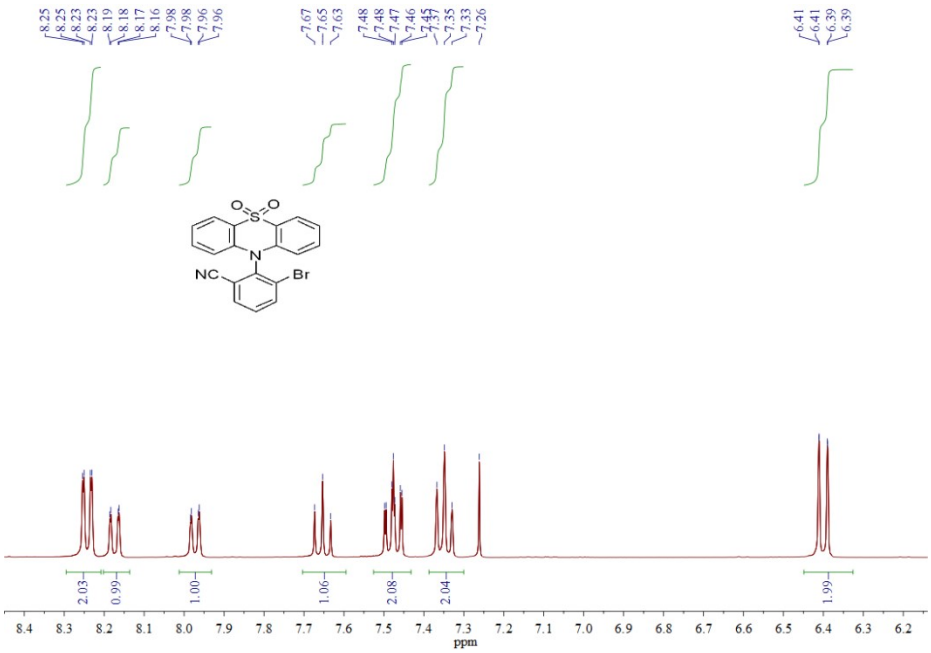
4.7 ^{1}H NMR plot of **5**, 400 MHz, $CDCl_3$



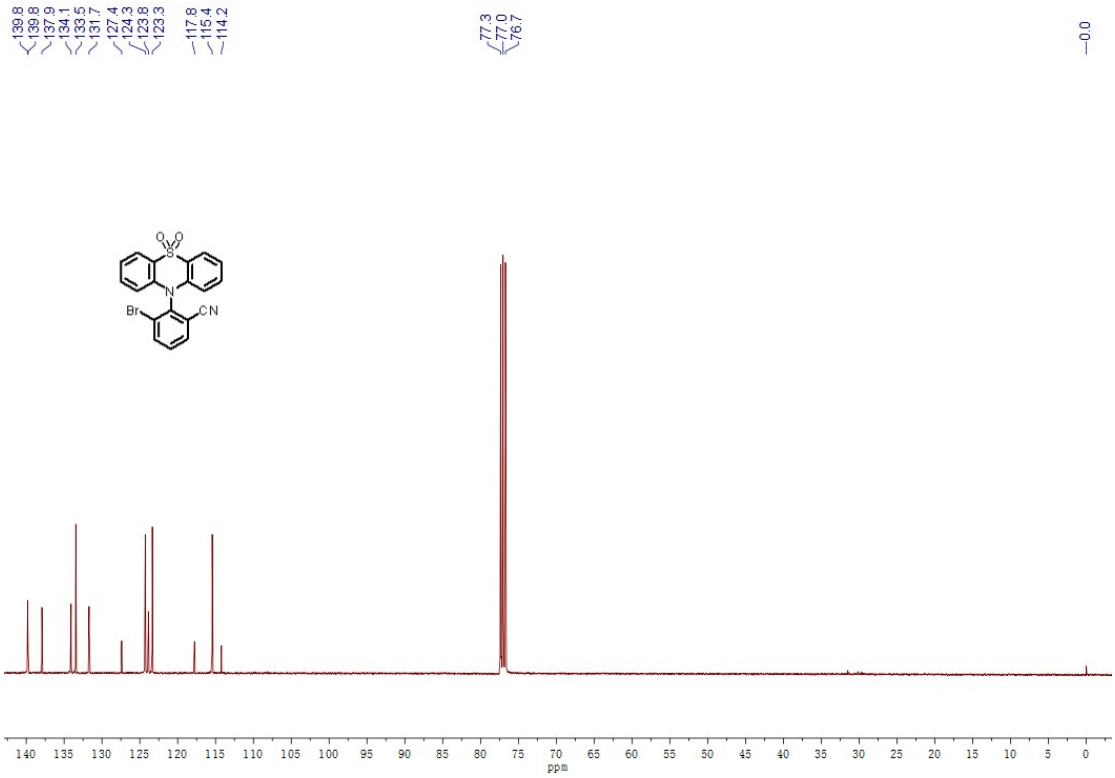
4.8 ^{13}C NMR plot of **5**, 101 MHz, $CDCl_3$



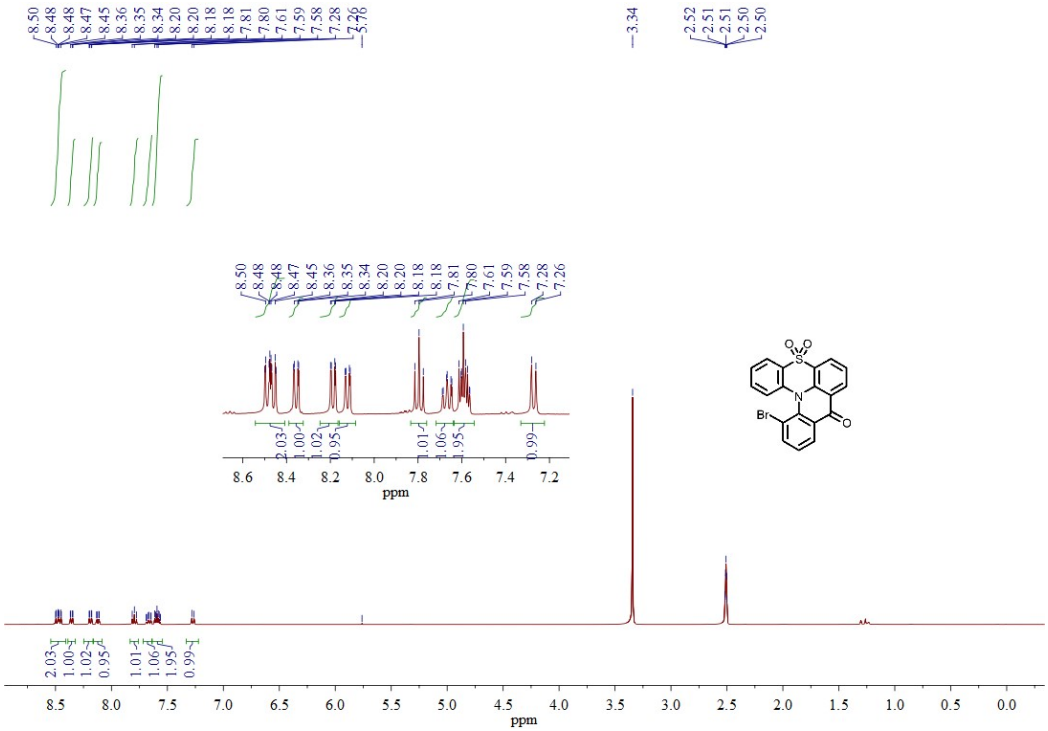
4.9 ^{1}H NMR plot of **6**, 400 MHz, $CDCl_3$



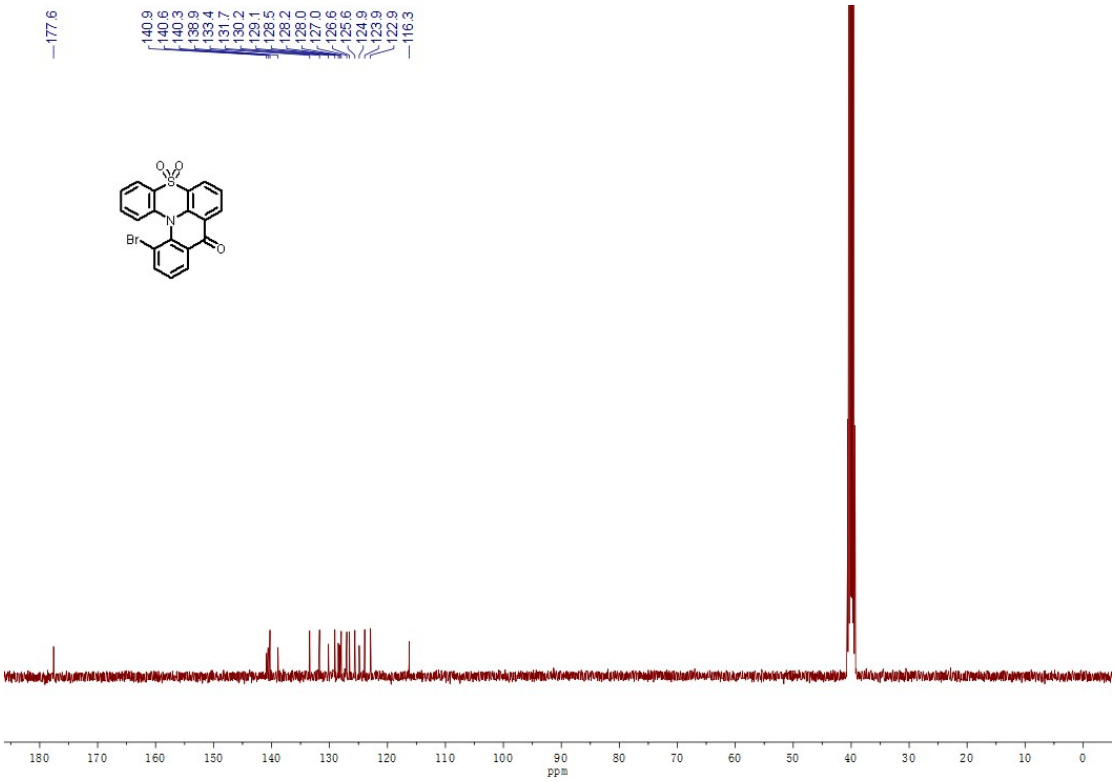
4.10 ^{13}C NMR plot of **6**, 101 MHz, $CDCl_3$



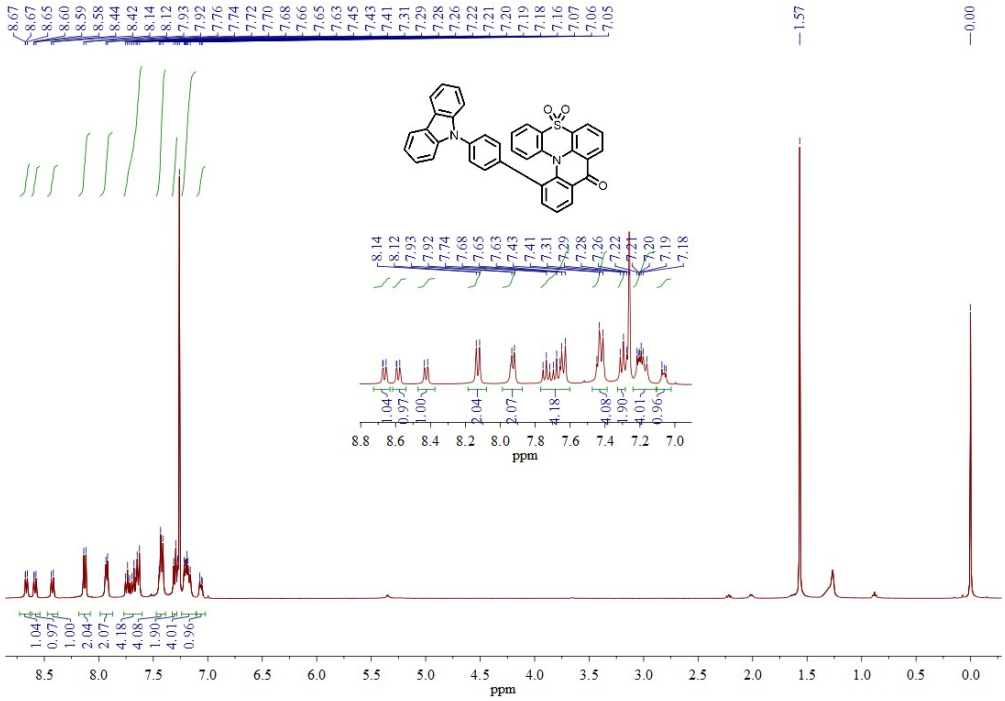
4.11 ^{1}H NMR plot of **QPO-Br**, 400 MHz, DMSO



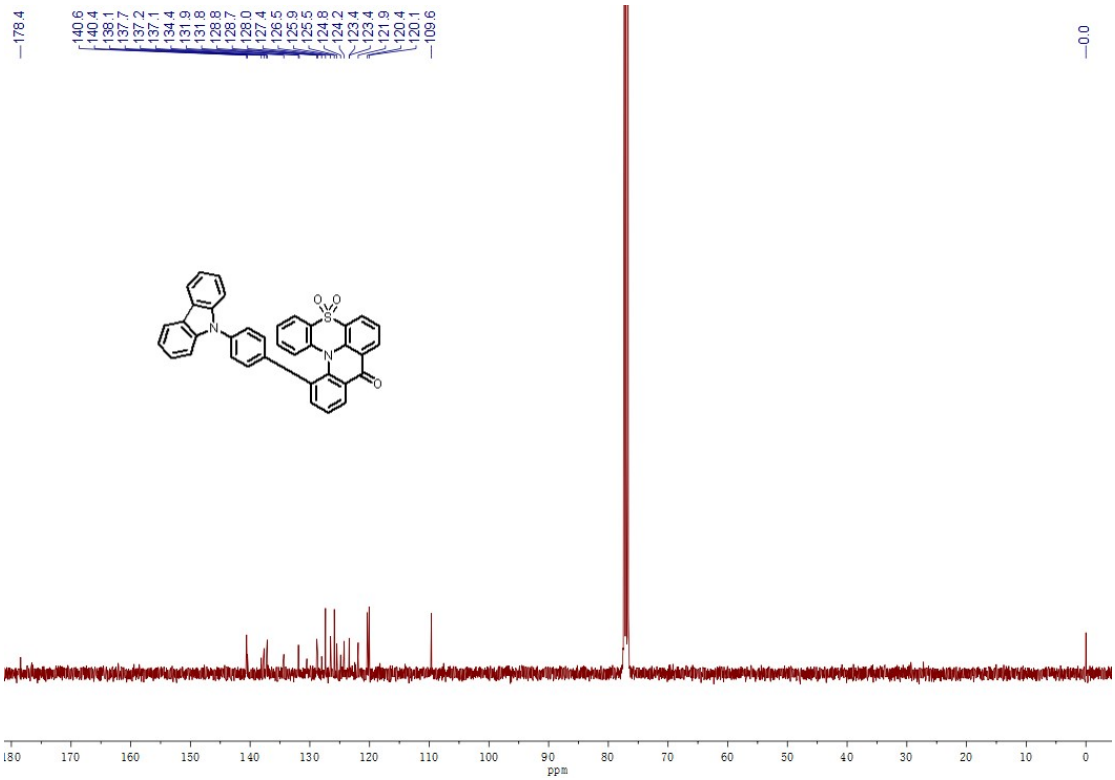
4.12 ^{13}C NMR plot of **QPO-Br**, 101 MHz, DMSO



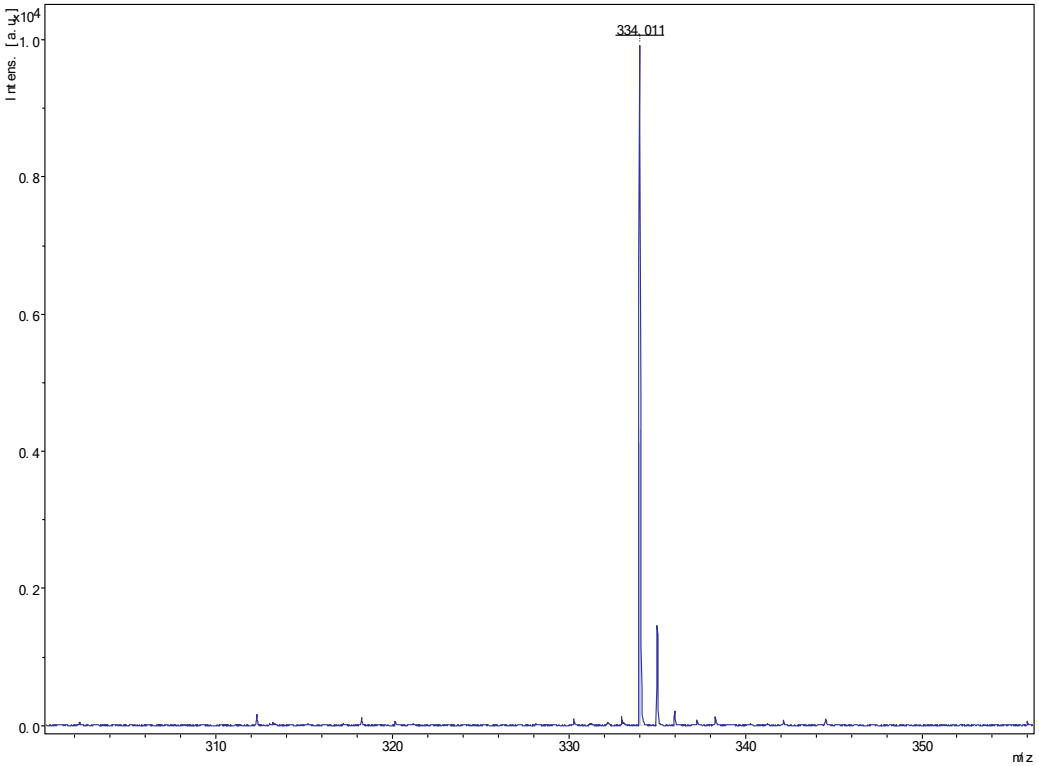
4.13 ^{1}H NMR plot of **QPO-PhCz**, 400 MHz, $CDCl_3$



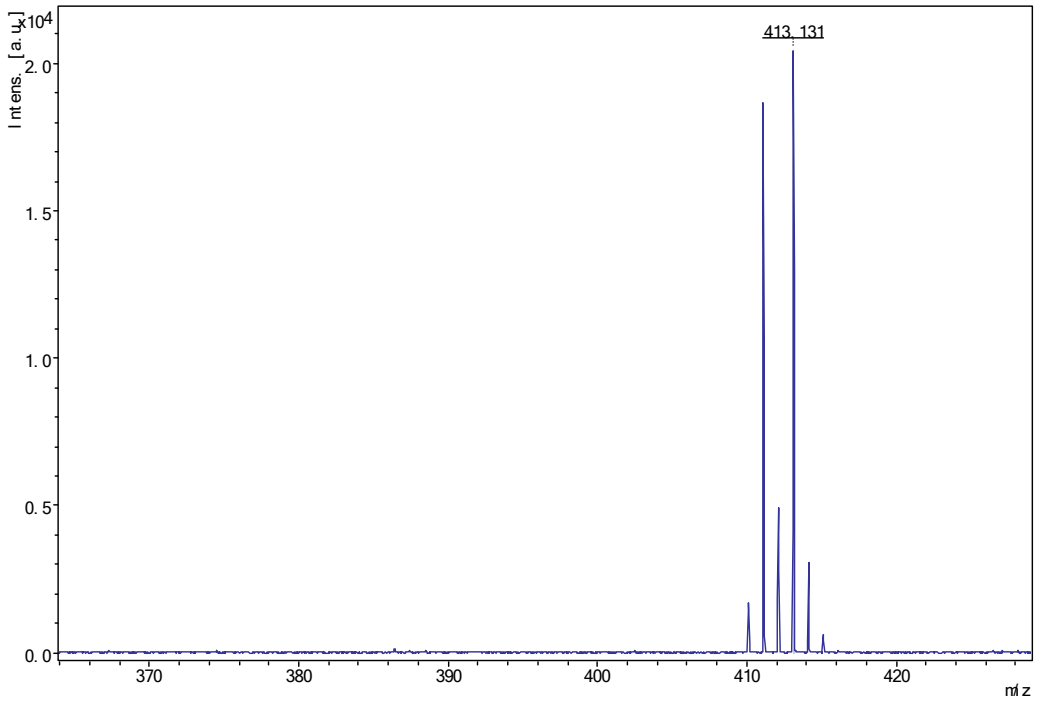
4.14 ^{13}C NMR plot of **QPO-PhCz**, 101 MHz, $CDCl_3$



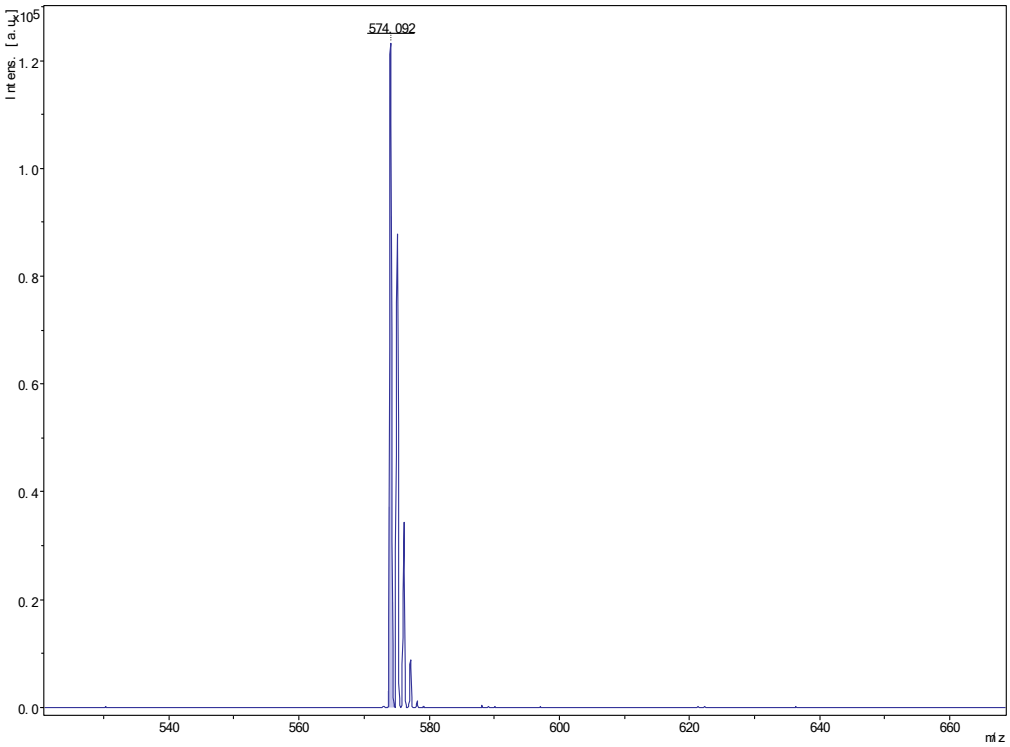
4.15 MALDI-TOF-MS plot of **QPO**



4.16 MALDI-TOF-MS plot of **QPO-Br**



4.17 MALDI-TOF-MS plot of **QPO-PhCz**



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