Electronic Supplementary Information (ESI)

A novel fluorene-based gold(I) complex with aggregate fluorescence change: a single-component white light-emitting luminophor

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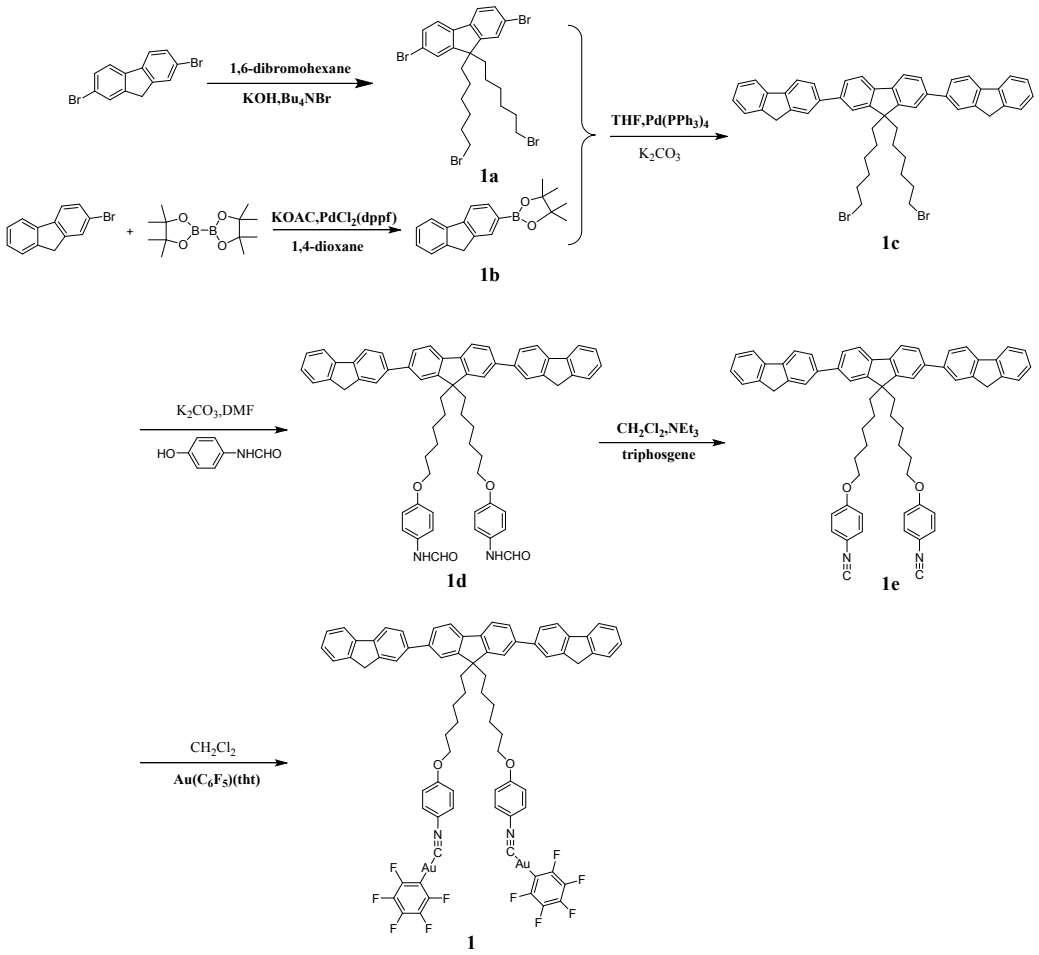
1. Experimental Section

Materials and measurements

All manipulations were carried out under an argon atmosphere by using standard Schlenk techniques, unless otherwise stated. The starting material 2, 7-dibromofluorene purchased from Alfa Aesar was used as received. DMF was dried with magnesum sulfate then distilled under vacuum, CH_2Cl_2 was dried with CaH_2 then distilled, and ultra-pure water was used in the experiments. All other starting materials and reagents were purchased as analytical-grade from Shen Shi Hua Gong Company (China) and used without further purification. Compounds **1a**[1], **1b**[2] N-(4-hydroxyphenyl)formamide[3] and $C_6F_5Au(tht)$[4] were prepared by procedures described in the corresponding literatures. ^1H NMR (400 MHz) and ^{13}C NMR (100.6 MHz) spectra were collected on American Varian Mercury Plus 400 spectrometer (400 MHz). ^1H NMR spectra are reported as followed: chemical shift in ppm (δ) relative to the chemical shift of TMS at 0.00 ppm, integration, multiplicities (s=singlet, d=doublet, t=triplet, m=multiplet), and coupling constant (Hz). ^{13}C NMR chemical shifts reported in ppm (δ) relative to the central line of triplet for $CDCl_3$ at 77 ppm. ^{19}F NMR chemical shifts are relative to C_6F_6 (δ= -163.00). EI-MS was obtained using Thermo scientific DSQⅡ. Elemental analyses (C, H, N) were performed by the Microanalytical Services, College of Chemistry, CCNU. UV-Vis spectra were obtained on U-3310 UV Spectrophotometer. Fluorescence spectra were recorded on a Hitachi-F-4500 fluorescence spectrophotometer and Fluoromax-P luminescence spectrometer (HORIBA JOBIN YVON INC.). the absolute fluorescence quantum yield was measured by Edinburgh Instruments FLS900. Dynamic light scattering (DLS) measurements were performed on the Zetasizer instrument ZEN3600 (Malvern, UK) with a 173° back scattering angle and He-Ne laser (λ =633 nm). The X-ray crystal-structure determinations of complex **1** was obtained on a Bruker APEX DUO CCD system.

The DMF/water mixtures with various water fractions were prepared by slowly

adding ultra-pure water into the DMF solution of samples.



Scheme S1. Synthesis of the complex **1**

General procedure for the synthesis

Synthesis of **1c:** A mixture of compounds **1a** (3.8 mmol, 2.5 g)，**1b** (9.6 mmol), K_2CO_3 (28.8 mmol), $Pd(PPh_3)_4$ (0.04 mmol) were stirred in THF (50 ml) and H_2O (5 ml) for two days under an argon atmosphere at 80℃. After completion of present reaction, the mixture was extracted with dichloromethane (3×20 mL). The combined organic layers were washed with brine, dried (Na_2SO_4), and concentrated in vacuo. The residues were purified by column chromatography, affording the expected white solid product in a yield of 60%. ^{1}H NMR (400 MH_Z, $CDCl_3$): δ (ppm)= 7.89-7.79 (m, 8H), 7.72-7.66 (m, 4H), 7.63 (s, 2H), 7.58 (d, J= 8 Hz, 2H), 7.40 (d, J= 8 Hz, 2H), 7.34 (d, J= 8 Hz, 2H), 4.01 (s, 4H), 3.27 (t, J= 6 Hz, 4H), 2.10 (s, 4H), 1.65 (d, J= 8 Hz, 4H), 1.23 (s, 4H), 1.12 (s, 4H), 0.76 (s, 4H). ^{13}C NMR

(100 MH_Z, $CDCl_3$): δ (ppm)= 151.31, 143.93, 143.42, 141.38, 140.88, 140.38, 140.13, 139.97, 126.80, 126.69, 126.22, 125.99, 125.02, 123.70, 121.30, 120.10, 119.93, 55.19, 40.27, 37.01, 33.81, 32.60, 29.01, 27.70, 23.62. EI-MS: m/z= 820.63$[M]^+$. Anal. Calcd. for $C_{51}H_{48}Br_2$: C, 74.63; H, 5.89. Found: C, 74.69; H, 5.85.

Synthesis of **1d:** A mixture of compounds **1c** (1.8 mmol, 1.5 g), N-(4-hydroxyphenyl)formamide (5.5 mmol), K_2CO_3 (21.9 mmol) were stirred in DMF (50 ml) for overnight under an argon atmosphere at 60℃. After completion of present reaction, DMF was removed from reaction system by vacuum distillation. the residual mixture was extracted with dichloromethane (3×20 mL). The combined organic layers were washed with brine, dried (Na_2SO_4), and concentrated in vacuo. The residues were purified by column chromatography, affording the expected yellow solid product in a yield of 58%. ^{1}H NMR (400 MH_Z, $CDCl_3$): δ (ppm)= 8.39 (d, J= 12 Hz, 1H), 8.21 (s, 1H), 7.84-7.65 (m, 13H), 7.56 (d, J= 8 Hz, 2H), 7.40-7.24 (m, 8H), 7.12 (d, J= 12 Hz, 1H), 6.86 (d, J= 8 Hz, 2H), 6.71 (d, J= 8 Hz, 4H), 3.94 (s, 4H), 3.74 (d, J= 4 Hz, 4H), 2.11 (s, 4H), 1.54 (s, 4H), 1.25 (d, J= 4 Hz, 4H), 1.16 (d, J= 4 Hz, 4H), 0.79 (s, 4H). ^{13}C NMR (100 MH_Z, $CDCl_3$): δ (ppm)= 162.64, 158.57, 151.46, 143.98, 143.47, 141.42, 140.87, 140.28, 129.05, 126.87, 126.17, 126.01, 125.10, 123.72, 121.65, 121.42, 120.10, 119.97, 115.44, 114.86, 68.21, 55.31, 40.25, 37.03, 29.50, 28.98, 25.49, 23.64. EI-MS: m/z= 933.71$[M]^+$. Anal. Calcd. for $C_{65}H_{60}N_2O_4$: C, 83.66; H, 6.48; N, 3.00. Found: C, 83.70; H, 6.40; N, 3.02.

Synthesis of **1e:** A CH_2Cl_2 suspension (15 ml) of **1d** (0.60 g, 0.64 mmol) and triethylamine (5 ml) was cooled to 0℃. To the mixture was added dropwise a CH_2Cl_2 solution (10 ml) of triphosgene (0.42 g, 1.42 mmol). The mixture was refluxed for 3 h, then 10% aq. Na_2CO_3 (50 ml) was added dropwise at room temperature. the mixture was extracted with dichloromethane (3×20 mL). The combined organic layers were washed with brine, dried (Na_2SO_4), and concentrated in vacuo. The residues were purified by column chromatography, affording the expected yellow solid product in a yield of 71%. ^{1}H NMR (400 MH_Z, $CDCl_3$): δ (ppm)= 7.85-7.79 (m, 8H), 7.70-7.64 (m,

6H), 7.58 (d, J= 8 Hz, 2H), 7.41 (d, J= 8 Hz, 2H), 7.35 (d, J= 8 Hz, 2H), 7.18 (d, J= 4 Hz, 4H), 6.70 (d, J= 8 Hz, 4H), 3.96 (s, 4H), 3.75 (d, J= 8 Hz, 4H), 2.11 (s, 4H), 1.56 (s, 4H), 1.23 (s, 4H), 1.15 (s, 4H), 0.77 (s, 4H). ^{13}C NMR (100 MHz, $CDCl_3$): δ (ppm)= 162.72, 159.36, 151.37, 143.97, 143.39, 141.32, 140.97, 140.37, 140.14, 140.08, 127.59, 126.93, 126.19, 125.95, 125.08, 123.67, 121.36, 120.12, 119.96, 114.94, 68.27, 55.27, 40.32, 37.03, 29.68, 28.83, 25.46, 23.67. EI-MS: m/z= 897.09[M]$^+$. Anal. Calcd. for $C_{65}H_{56}N_2O_2$: C, 87.02; H, 6.29; N, 3.12. Found: C, 87.05; H, 6.35; N, 3.05.

Synthesis of **1:** A mixture of $C_6F_5Au(tht)$ (0.21 g, 0.46 mmol) and **1e** (0.2 g, 0.22 mmol) was stirred in CH_2Cl_2 (20 ml) over night under an argon atmosphere at room temperature. After completion of present reaction, the solvent was evaporated. A small amount of CH_2Cl_2 was added, and then a lot of n-hexane was added. Collecting the white solid product by suction filtration. Yield= 91%. ^{1}H NMR (400 MHz，$CDCl_3$): δ (ppm)= 7.81 (t, J= 12 Hz, 9H), 7.68 (t, J= 8 Hz, 6H), 7.58 (d, J= 4 Hz, 2H), 7.43 (t, J= 8 Hz, 2H), 7.35 (t, J= 8 Hz, 2H), 7.22 (t, J= 8 Hz, 3H), 6.72 (d, J= 12 Hz, 4H), 3.94 (s, 4H), 3.76 (t, J= 6 Hz, 4H), 2.13 (s, 4H), 1.55 (s, 4H), 1.16 (d, J= 8 Hz, 4H), 0.88 (t, J= 8 Hz, 4H), 0.78 (s, 4H). ^{19}F NMR ($CDCl_3$): δ (ppm)= -116.95, -158.37, -163.21. Anal. Calcd for $C_{77}H_{56}Au_2F_{10}N_2O_2$： C, 56.91; H, 3.47; N, 1.72. Found: C, 57.02; H, 3.42; N, 1.63.

Crystallographic Details

Single crystals of complex **1** suitable for X-ray analysis were obtained by slow diffusion of *n*-hexane into a solution of dichloromethane. A crystal of **1** with approximate dimensions of 0.10 × 0.10 × 0.10 mm^3 for **1** was mounted on a glass fiber for diffraction experiment. Intensity data were collected on a Nonius Kappa CCD diffractometer with Mo Kα radiation (0.71073 Å) at room temperature. The structures were solved by a combination of direct methods (SHELXS-97)[5] and Fourier difference techniques and refined by full-matrix least-squares (SHELXL-97)[6]. All non-H atoms were refined anisotropically. The hydrogen

atoms were placed in the ideal positions and refined as riding atoms. Further crystal data is summarized in Table S1. Selected bond distances and angles is given in Table S2. Crystallographic data for the structure in this paper have been deposited with the Cambridge Crystallographic Data Centre as supplemental publication CCDC 1002798.

2. References

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6. G. M. Sheldrick, SHELXL-97: Program for crystal structure refinement, University of Götingen, Götingen, Germany, **1997**.

3. Figs. S1-S3

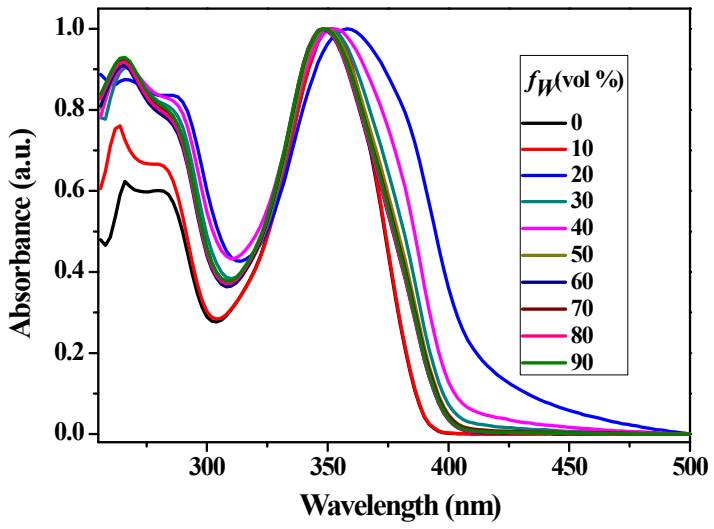


Fig. S1 UV spectra of complex **1** (2.0×10^{-5} mol L^{-1}) in water-DMF mixtures with various volume fractions of water (0-90%).

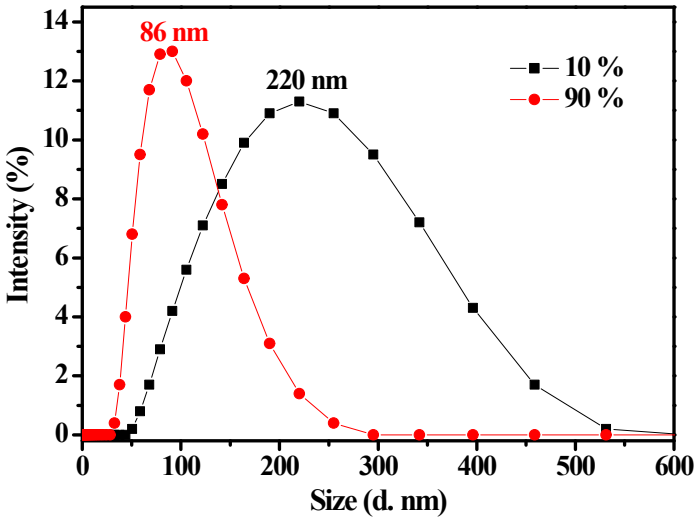


Fig. S2 Size distribution curves of complex **1** (2.0×10^{-5} mol L^{-1}) in water-DMF mixtures with different volume fractions of water (10% and 90%).

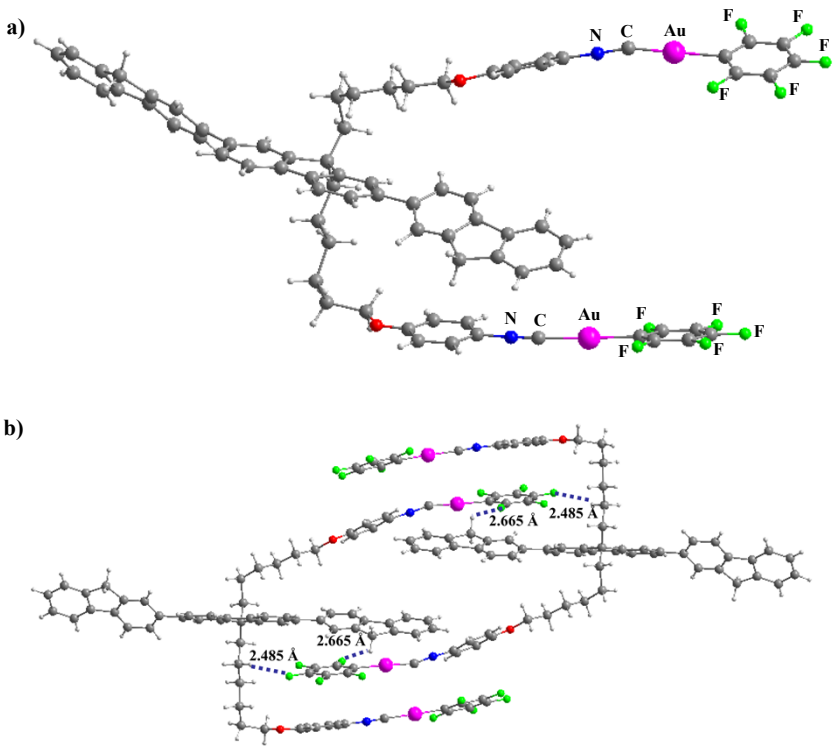


Fig. S3 a) The single crystal structure of complex **1**. b) Crystal packing diagram of complex **1**. It showed weak interactions of intermolecular C-H···F.

4. Table S1-S2

Table S1. Structure determination summary for the complex **1**.

Empirical formula	$C_{77}\ H_{56}\ Au_2\ F_{10}\ N_2\ O_2$
Formula weight	1625.17
Temperature (K)	100(2)
Crystal system	Triclinic
Space group	P-1
a (Å)	11.9116(16)
b (Å)	12.7221(17)
c (Å)	21.939(3)
α (deg)	92.367(9)
β (deg)	90.803(9)
γ (deg)	102.203(8)
V (Å^3)	3245.8(8)
Z	2
Absorption coefficient (mm^{-1})	9.039
F (000)	1592
Theta range for data collection (deg)	2.02 to 43.40
Index ranges	-10<=h<=10, -11<=k<=11, -19<=l<=19
Reflections collected/unique	21688/4569 (R_{int}= 0.2465)
Final R indices [I>2sigma(I)]	R_1= 0.1066, wR_2= 0.2691
R indices (all data)	R_1= 0.2354, wR_2= 0.3093
Goodness-of-fit on F^2	1.161
Largest difference peak and hole(e Å^{-3})	2.444, -1.083

Table S2. Selective bond lengths [Å] and angles [°] of **1**.

Au(1)-C(7)	2.01(4)	C(1)-C(2)	1.3900
Au(1)-C(1)	2.029(16)	C(1)-C(6)	1.3900
Au(2)-C(32)	1.83(5)	C(2)-F(1)	1.30(2)
Au(2)-C(72)	2.071(19)	C(2)-C(3)	1.3900

C(3)-F(2)	1.34(3)	C(19)-H(19B)	0.9900
C(3)-C(4)	1.3900	C(20)-C(33)	1.52(4)
C(4)-F(3)	1.37(2)	C(20)-C(21)	1.58(4)
C(4)-C(5)	1.3900	C(20)-H(20A)	0.9900
C(5)-F(4)	1.38(2)	C(20)-H(20B)	0.9900
C(5)-C(6)	1.3900	C(21)-C(22)	1.50(4)
C(6)-F(5)	1.33(3)	C(21)-H(21A)	0.9900
C(7)-N(1)	1.13(3)	C(21)-H(21B)	0.9900
C(8)-C(9)	1.3900	C(22)-C(23)	1.49(4)
C(8)-C(13)	1.3900	C(22)-H(22A)	0.9900
C(8)-N(1)	1.39(3)	C(22)-H(22B)	0.9900
C(9)-C(10)	1.3900	C(23)-C(24)	1.48(4)
C(9)-H(9)	0.9500	C(23)-H(23A)	0.9900
C(10)-C(11)	1.3900	C(23)-H(23B)	0.9900
C(10)-H(10)	0.9500	C(24)-C(25)	1.42(4)
C(11)-O(1)	1.29(2)	C(24)-H(24A)	0.9900
C(11)-C(12)	1.3900	C(24)-H(24B)	0.9900
C(12)-C(13)	1.3900	C(25)-O(2)	1.47(4)
C(12)-H(12)	0.9500	C(25)-H(25A)	0.9900
C(13)-H(13)	0.9500	C(25)-H(25B)	0.9900
C(14)-O(1)	1.33(3)	C(26)-O(2)	1.37(3)
C(14)-C(15)	1.61(4)	C(26)-C(27)	1.3900
C(14)-H(14A)	0.9900	C(26)-C(31)	1.3900
C(14)-H(14B)	0.9900	C(27)-C(28)	1.3900
C(15)-C(16)	1.49(5)	C(27)-H(27)	0.9500
C(15)-H(15A)	0.9900	C(28)-C(29)	1.3900
C(15)-H(15B)	0.9900	C(28)-H(28)	0.9500
C(16)-C(17)	1.62(4)	C(29)-C(30)	1.3900
C(16)-H(16A)	0.9900	C(29)-N(2)	1.41(4)
C(16)-H(16B)	0.9900	C(30)-C(31)	1.3900
C(17)-C(18)	1.49(4)	C(30)-H(30)	0.9500
C(17)-H(17A)	0.9900	C(31)-H(31)	0.9500
C(17)-H(17B)	0.9900	C(33)-C(34)	1.54(3)
C(18)-C(19)	1.54(4)	C(33)-C(37)	1.55(3)
C(18)-H(18A)	0.9900	C(35)-C(34)	1.3900
C(18)-H(18B)	0.9900	C(35)-C(41)	1.3900
C(19)-C(33)	1.54(4)	C(35)-C(36)	1.46(2)
C(19)-H(19A)	0.9900	C(34)-C(38)	1.3900

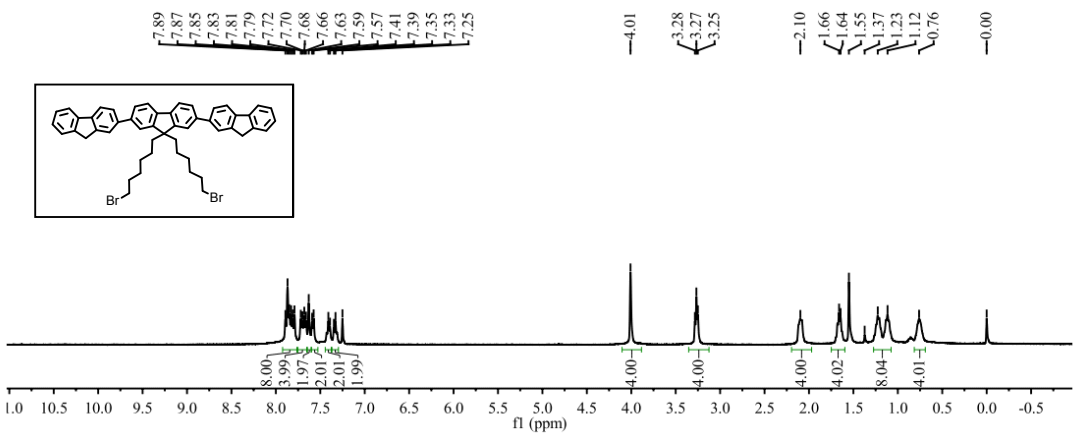
C(38)-C(39)	1.3900	C(12)-C(13)-C(8)	120.0
C(38)-H(38)	0.9500	C(12)-C(13)-H(13)	120.0
C(7)-Au(1)-C(1)	176.9(12)	C(8)-C(13)-H(13)	120.0
C(32)-Au(2)-C(72)	176.8(18)	O(1)-C(14)-C(15)	111(3)
C(2)-C(1)-C(6)	120.0	O(1)-C(14)-H(14A)	109.5
C(2)-C(1)-Au(1)	121.6(18)	C(15)-C(14)-H(14A)	109.5
C(6)-C(1)-Au(1)	118.4(19)	O(1)-C(14)-H(14B)	109.5
F(1)-C(2)-C(3)	120(2)	C(15)-C(14)-H(14B)	109.5
F(1)-C(2)-C(1)	120(2)	H(14A)-C(14)-H(14B)	108.0
C(3)-C(2)-C(1)	120.0	C(16)-C(15)-C(14)	115(3)
F(2)-C(3)-C(2)	119(2)	C(16)-C(15)-H(15A)	108.4
F(2)-C(3)-C(4)	121(2)	C(14)-C(15)-H(15A)	108.4
C(2)-C(3)-C(4)	120.0	C(16)-C(15)-H(15B)	108.4
F(3)-C(4)-C(5)	124(2)	C(14)-C(15)-H(15B)	108.4
F(3)-C(4)-C(3)	116(2)	H(15A)-C(15)-H(15B)	107.5
C(5)-C(4)-C(3)	120.0	C(15)-C(16)-C(17)	113(3)
F(4)-C(5)-C(4)	115(2)	C(15)-C(16)-H(16A)	108.9
F(4)-C(5)-C(6)	125(2)	C(17)-C(16)-H(16A)	108.9
C(4)-C(5)-C(6)	120.0	C(15)-C(16)-H(16B)	108.9
F(5)-C(6)-C(5)	112(2)	C(17)-C(16)-H(16B)	108.9
F(5)-C(6)-C(1)	128(2)	H(16A)-C(16)-H(16B)	107.7
C(5)-C(6)-C(1)	120.0	C(18)-C(17)-C(16)	113(3)
N(1)-C(7)-Au(1)	170(3)	C(18)-C(17)-H(17A)	109.0
C(9)-C(8)-C(13)	120.0	C(16)-C(17)-H(17A)	109.0
C(9)-C(8)-N(1)	120(2)	C(18)-C(17)-H(17B)	109.0
C(13)-C(8)-N(1)	120(2)	C(16)-C(17)-H(17B)	109.0
C(8)-C(9)-C(10)	120.0	H(17A)-C(17)-H(17B)	107.8
C(8)-C(9)-H(9)	120.0	C(17)-C(18)-C(19)	108(3)
C(10)-C(9)-H(9)	120.0	C(17)-C(18)-H(18A)	110.0
C(9)-C(10)-C(11)	120.0	C(19)-C(18)-H(18A)	110.0
C(9)-C(10)-H(10)	120.0	C(17)-C(18)-H(18B)	110.0
C(11)-C(10)-H(10)	120.0	C(19)-C(18)-H(18B)	110.0
O(1)-C(11)-C(12)	117(2)	H(18A)-C(18)-H(18B)	108.4
O(1)-C(11)-C(10)	123(2)	C(33)-C(19)-C(18)	114(3)
C(12)-C(11)-C(10)	120.0	C(33)-C(19)-H(19A)	108.7
C(11)-C(12)-C(13)	120.0	C(18)-C(19)-H(19A)	108.7
C(11)-C(12)-H(12)	120.0	C(33)-C(19)-H(19B)	108.7
C(13)-C(12)-H(12)	120.0	C(18)-C(19)-H(19B)	108.7

H(19A)-C(19)-H(19B)	107.6	O(2)-C(26)-C(31)	113(3)
C(33)-C(20)-C(21)	117(3)	C(27)-C(26)-C(31)	120.0
C(33)-C(20)-H(20A)	108.1	C(28)-C(27)-C(26)	120.0
C(21)-C(20)-H(20A)	108.1	C(28)-C(27)-H(27)	120.0
C(33)-C(20)-H(20B)	108.1	C(26)-C(27)-H(27)	120.0
C(21)-C(20)-H(20B)	108.1	C(27)-C(28)-C(29)	120.0
H(20A)-C(20)-H(20B)	107.3	C(27)-C(28)-H(28)	120.0
C(22)-C(21)-C(20)	123(3)	C(29)-C(28)-H(28)	120.0
C(22)-C(21)-H(21A)	106.6	C(30)-C(29)-C(28)	120.0
C(20)-C(21)-H(21A)	106.6	C(30)-C(29)-N(2)	117(3)
C(22)-C(21)-H(21B)	106.6	C(28)-C(29)-N(2)	122(3)
C(20)-C(21)-H(21B)	106.6	C(29)-C(30)-C(31)	120.0
H(21A)-C(21)-H(21B)	106.6	C(29)-C(30)-H(30)	120.0
C(23)-C(22)-C(21)	107(3)	C(31)-C(30)-H(30)	120.0
C(23)-C(22)-H(22A)	110.3	C(30)-C(31)-C(26)	120.0
C(21)-C(22)-H(22A)	110.3	C(30)-C(31)-H(31)	120.0
C(23)-C(22)-H(22B)	110.3	C(26)-C(31)-H(31)	120.0
C(21)-C(22)-H(22B)	110.3	C(20)-C(33)-C(19)	106(3)
H(22A)-C(22)-H(22B)	108.6	C(20)-C(33)-C(34)	113(3)
C(24)-C(23)-C(22)	111(3)	C(19)-C(33)-C(34)	111(2)
C(24)-C(23)-H(23A)	109.4	C(20)-C(33)-C(37)	112(2)
C(22)-C(23)-H(23A)	109.4	C(19)-C(33)-C(37)	116(2)
C(24)-C(23)-H(23B)	109.4	C(34)-C(33)-C(37)	98(2)
C(22)-C(23)-H(23B)	109.4	C(34)-C(35)-C(41)	120.0
H(23A)-C(23)-H(23B)	108.0	C(34)-C(35)-C(36)	110(2)
C(25)-C(24)-C(23)	118(3)	C(41)-C(35)-C(36)	130(2)
C(25)-C(24)-H(24A)	107.9	C(35)-C(34)-C(38)	120.0
C(23)-C(24)-H(24A)	107.9	C(35)-C(34)-C(33)	111(2)
C(25)-C(24)-H(24B)	107.9	C(38)-C(34)-C(33)	129(2)
C(23)-C(24)-H(24B)	107.9	C(39)-C(38)-C(34)	120.0
H(24A)-C(24)-H(24B)	107.2	C(39)-C(38)-H(38)	120.0
C(24)-C(25)-O(2)	114(3)	C(34)-C(38)-H(38)	120.0
C(24)-C(25)-H(25A)	108.8	C(38)-C(39)-C(40)	120.0
O(2)-C(25)-H(25A)	108.8	C(38)-C(39)-C(42)	120(2)
C(24)-C(25)-H(25B)	108.8	C(40)-C(39)-C(42)	120(2)
O(2)-C(25)-H(25B)	108.8	C(41)-C(40)-C(39)	120.0
H(25A)-C(25)-H(25B)	107.7	C(41)-C(40)-H(40)	120.0
O(2)-C(26)-C(27)	127(3)	C(39)-C(40)-H(40)	120.0

C(40)-C(41)-C(35)	120.0	C(48)-C(54)-H(54)	120.0
C(40)-C(41)-H(41)	120.0	C(49)-C(50)-C(44)	97(3)
C(35)-C(41)-H(41)	120.0	C(49)-C(50)-H(50A)	112.4
C(47)-C(42)-C(43)	117(3)	C(44)-C(50)-H(50A)	112.4
C(47)-C(42)-C(39)	123(3)	C(49)-C(50)-H(50B)	112.4
C(43)-C(42)-C(39)	120(3)	C(44)-C(50)-H(50B)	112.4
C(44)-C(43)-C(42)	121(3)	H(50A)-C(50)-H(50B)	110.0
C(44)-C(43)-H(43)	119.7	C(36)-C(37)-C(58)	120.0
C(42)-C(43)-H(43)	119.7	C(36)-C(37)-C(33)	113(2)
C(43)-C(44)-C(45)	123(3)	C(58)-C(37)-C(33)	127(2)
C(43)-C(44)-C(50)	125(4)	C(37)-C(36)-C(55)	120.0
C(45)-C(44)-C(50)	112(3)	C(37)-C(36)-C(35)	107(2)
C(44)-C(45)-C(46)	119(3)	C(55)-C(36)-C(35)	133(2)
C(44)-C(45)-C(48)	111(3)	C(56)-C(55)-C(36)	120.0
C(46)-C(45)-C(48)	130(4)	C(56)-C(55)-H(55)	120.0
C(45)-C(46)-C(47)	117(3)	C(36)-C(55)-H(55)	120.0
C(45)-C(46)-H(46)	121.4	C(55)-C(56)-C(57)	120.0
C(47)-C(46)-H(46)	121.4	C(55)-C(56)-H(56)	120.0
C(42)-C(47)-C(46)	123(3)	C(57)-C(56)-H(56)	120.0
C(42)-C(47)-H(47)	118.6	C(58)-C(57)-C(56)	120.0
C(46)-C(47)-H(47)	118.6	C(58)-C(57)-C(59)	123(3)
C(49)-C(48)-C(54)	120.0	C(56)-C(57)-C(59)	117(3)
C(49)-C(48)-C(45)	107(3)	C(57)-C(58)-C(37)	120.0
C(54)-C(48)-C(45)	133(3)	C(57)-C(58)-H(58)	120.0
C(51)-C(49)-C(48)	120.0	C(37)-C(58)-H(58)	120.0
C(51)-C(49)-C(50)	127(2)	C(64)-C(59)-C(60)	118(2)
C(48)-C(49)-C(50)	113(2)	C(64)-C(59)-C(57)	121(4)
C(52)-C(51)-C(49)	120.0	C(60)-C(59)-C(57)	120(3)
C(52)-C(51)-H(51)	120.0	C(61)-C(60)-C(59)	119(3)
C(49)-C(51)-H(51)	120.0	C(61)-C(60)-H(60)	120.4
C(53)-C(52)-C(51)	120.0	C(59)-C(60)-H(60)	120.4
C(53)-C(52)-H(52)	120.0	C(60)-C(61)-C(62)	117(3)
C(51)-C(52)-H(52)	120.0	C(60)-C(61)-C(65)	130(4)
C(52)-C(53)-C(54)	120.0	C(62)-C(61)-C(65)	113(3)
C(52)-C(53)-H(53)	120.0	C(63)-C(62)-C(61)	121(3)
C(54)-C(53)-H(53)	120.0	C(63)-C(62)-C(67)	137(4)
C(53)-C(54)-C(48)	120.0	C(61)-C(62)-C(67)	102(3)
C(53)-C(54)-H(54)	120.0	C(62)-C(63)-C(64)	129(3)

C(62)-C(63)-H(63)	115.4	C(61)-C(65)-H(65B)	110.3
C(64)-C(63)-H(63)	115.4	C(66)-C(65)-H(65B)	110.3
C(63)-C(64)-C(59)	115(3)	H(65A)-C(65)-H(65B)	108.6
C(63)-C(64)-H(64)	122.5	C(73)-C(72)-C(77)	120.0
C(59)-C(64)-H(64)	122.5	C(73)-C(72)-Au(2)	120(2)
C(67)-C(66)-C(71)	120.0	C(77)-C(72)-Au(2)	120(2)
C(67)-C(66)-C(65)	106(3)	F(6)-C(73)-C(74)	116(3)
C(71)-C(66)-C(65)	134(3)	F(6)-C(73)-C(72)	124(3)
C(68)-C(67)-C(66)	120.0	C(74)-C(73)-C(72)	120.0
C(68)-C(67)-C(62)	129(3)	F(7)-C(74)-C(73)	125(3)
C(66)-C(67)-C(62)	111(3)	F(7)-C(74)-C(75)	115(3)
C(67)-C(68)-C(69)	120.0	C(73)-C(74)-C(75)	120.0
C(67)-C(68)-H(68)	120.0	F(8)-C(75)-C(74)	124(3)
C(69)-C(68)-H(68)	120.0	F(8)-C(75)-C(76)	116(3)
C(70)-C(69)-C(68)	120.0	C(74)-C(75)-C(76)	120.0
C(70)-C(69)-H(69)	120.0	F(9)-C(76)-C(75)	120(3)
C(68)-C(69)-H(69)	120.0	F(9)-C(76)-C(77)	120(3)
C(69)-C(70)-C(71)	120.0	C(75)-C(76)-C(77)	120.0
C(69)-C(70)-H(70)	120.0	F(10)-C(77)-C(76)	119(3)
C(71)-C(70)-H(70)	120.0	F(10)-C(77)-C(72)	121(3)
C(70)-C(71)-C(66)	120.0	C(76)-C(77)-C(72)	120.0
C(70)-C(71)-H(71)	120.0	C(7)-N(1)-C(8)	176(3)
C(66)-C(71)-H(71)	120.0	C(32)-N(2)-C(29)	174(4)
C(61)-C(65)-C(66)	107(3)	C(11)-O(1)-C(14)	119(2)
C(61)-C(65)-H(65A)	110.3	C(26)-O(2)-C(25)	115(3)
C(66)-C(65)-H(65A)	110.3	N(2)-C(32)-Au(2)	163(4)

5. Copies of NMR spectra and Mass spectra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7.66
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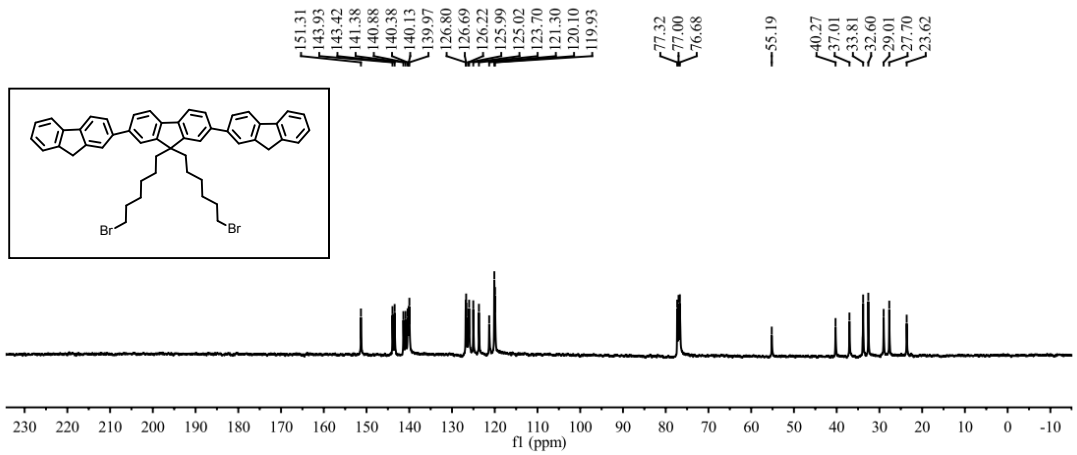
7.41
7.39
7.35
7.33
7.25
4.01
3.28
3.27
3.25
2.10
1.66
1.64
1.55
1.37
1.23
1.12
0.76
0.00
Br
Br
8.00
3.99
1.97
2.01
2.01
1.99
4.00
4.00
4.00
4.02
8.04
4.01
f1 (ppm)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139.97
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126.22
125.99
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123.70
121.30
120.10
119.93
77.32
77.00
76.68
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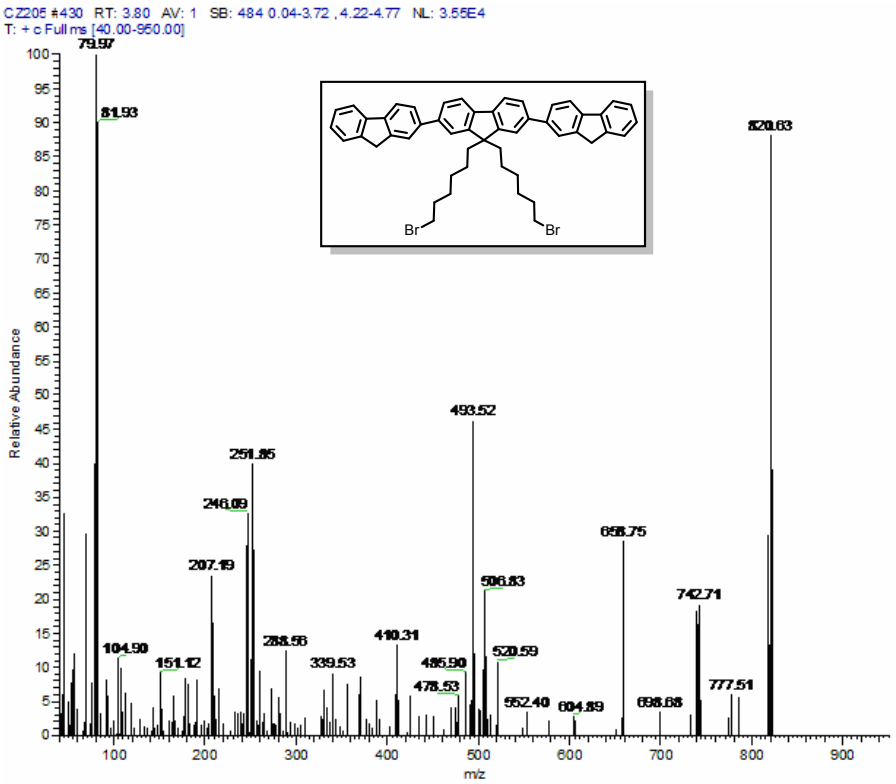
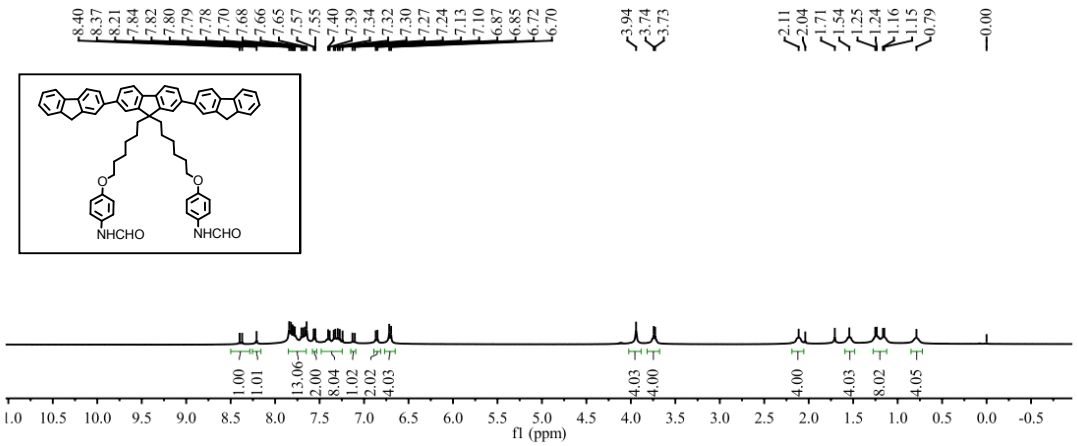
40.27
37.01
33.81
32.60
29.01
27.70
23.62
Br
Br
f1 (ppm)


CZ205 #430 RT: 3.80 AV: 1 SB: 484 0.04-3.72 , 4.22-4.77 NL: 3.55E4
T: + c Full ms [40.00-950.00]
79.97
81.93
820.63
493.52
251.85
246.09
658.75
207.19
506.83
742.71
104.90
288.56
410.31
151.12
339.53
485.90
520.59
478.53
552.40
604.89
698.68
777.51
Relative Abundance
m/z
Br
Br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7.79
7.78
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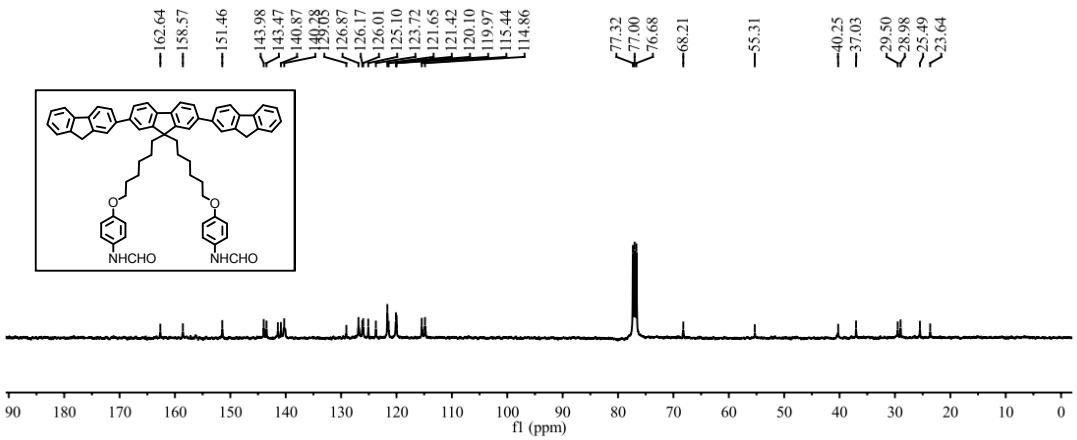
7.68
7.66
7.65
7.57
7.55
7.40
7.39
7.34
7.32
7.30
7.27
7.24
7.13
7.10
6.87
6.85
6.72
6.70
3.94
3.74
3.73
2.11
2.04
1.71
1.54
1.25
1.24
1.16
1.15
0.79
0.00
NHCHO
NHCHO
1.00
1.01
13.06
2.00
8.04
1.02
2.02
4.03
4.03
4.00
4.00
4.03
8.02
4.05
f1 (ppm)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140.87
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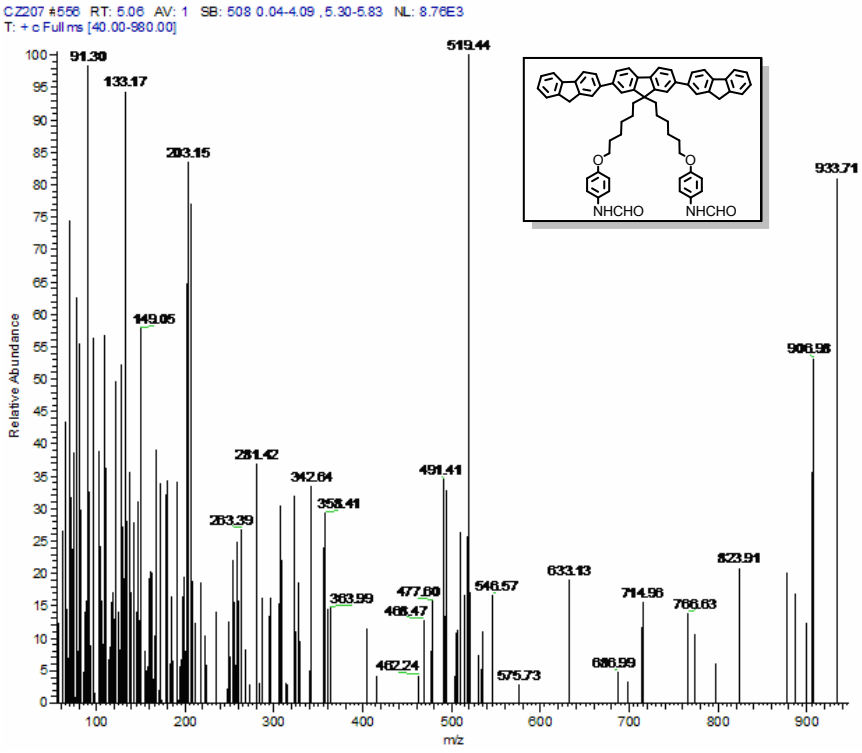
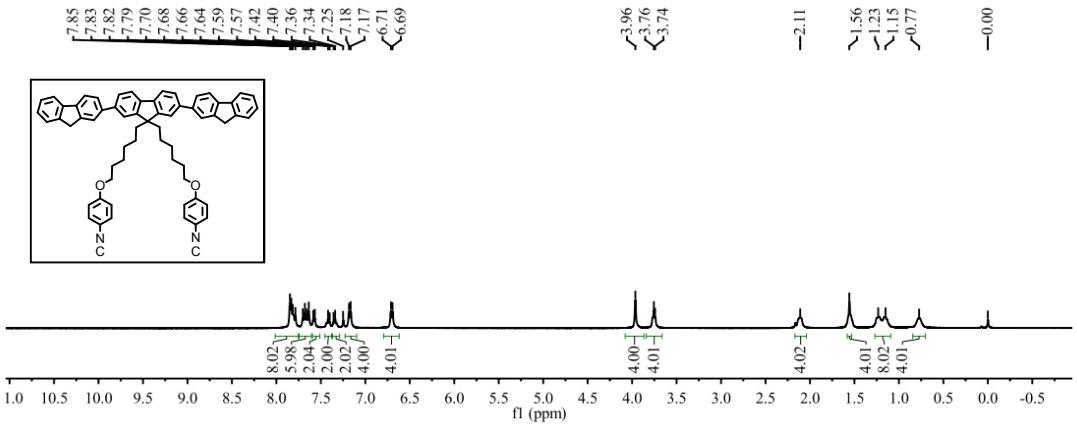
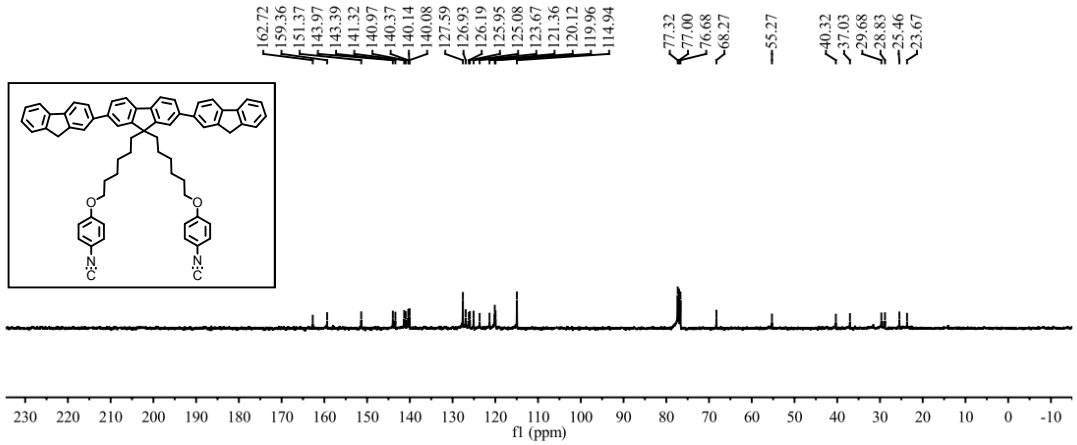
126.17
126.01
125.10
123.72
121.65
121.42
120.10
119.97
115.44
114.86
77.32
77.00
76.68
68.21
55.31
40.25
37.03
29.50
28.98
25.49
23.64
NHCHO
NHCHO
f1 (ppm)


CZ207 #556 RT: 5.06 AV: 1 SB: 508 0.04-4.09 , 5.30-5.83 NL: 8.76E3
T: + c Full ms [40.00-980.00]
Relative Abundance
m/z
91.30
133.17
203.15
149.05
281.42
342.64
358.41
263.39
363.99
477.60
468.47
462.24
491.41
519.44
546.57
575.73
633.13
686.99
714.96
766.63
823.91
906.96
933.71
NHCHO
NHCHO


7.85
7.83
7.82
7.79
7.70
7.68
7.66
7.64
7.59
7.57
7.42
7.40
7.36
7.34
7.25
7.18
7.17
6.71
6.69
3.96
3.76
3.74
2.11
1.56
1.23
1.15
0.77
0.00
8.02
5.98
2.04
2.00
2.02
4.00
4.01
4.00
4.01
4.02
4.01
8.02
4.01
fl (ppm)


162.72
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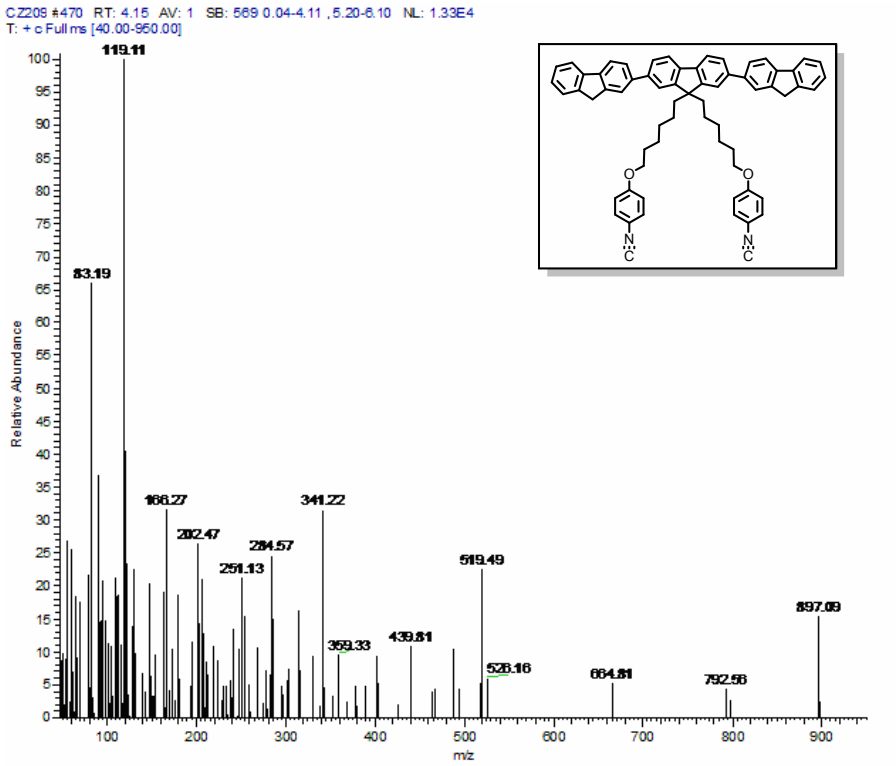
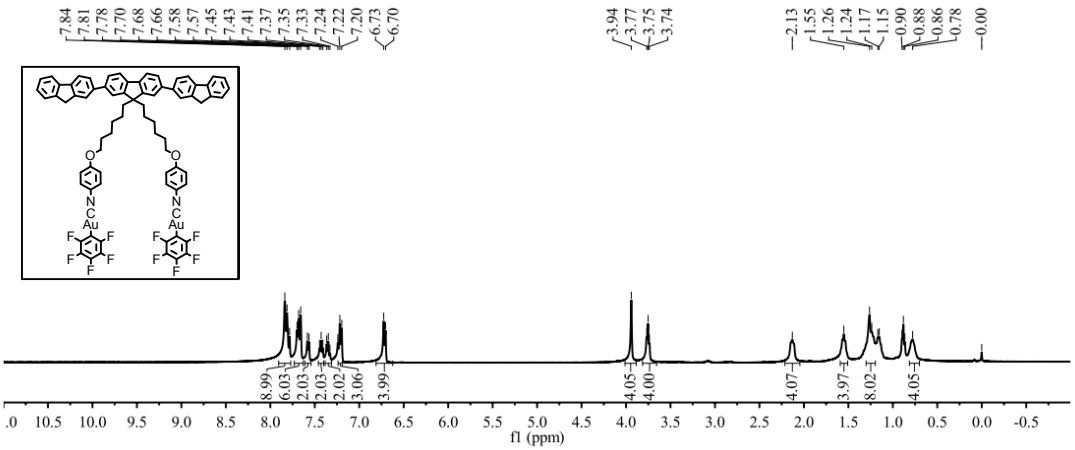
151.37
143.97
143.39
141.32
140.97
140.37
140.14
140.08
127.59
126.93
126.19
125.95
125.08
123.67
121.36
120.12
119.96
114.94
77.32
77.00
76.68
68.27
55.27
40.32
37.03
29.68
28.83
25.46
23.67
fl (ppm)


CZ209 #470 RT: 4.15 AV: 1 SB: 569 0.04-4.11 , 5.20-6.10 NL: 1.33E4
T: + c Full ms [40.00-950.00]
Relative Abundance
m/z
119.11
83.19
166.27
202.47
284.57
251.13
341.22
359.33
439.61
519.49
526.16
664.81
792.56
897.09


7.84
7.81
7.78
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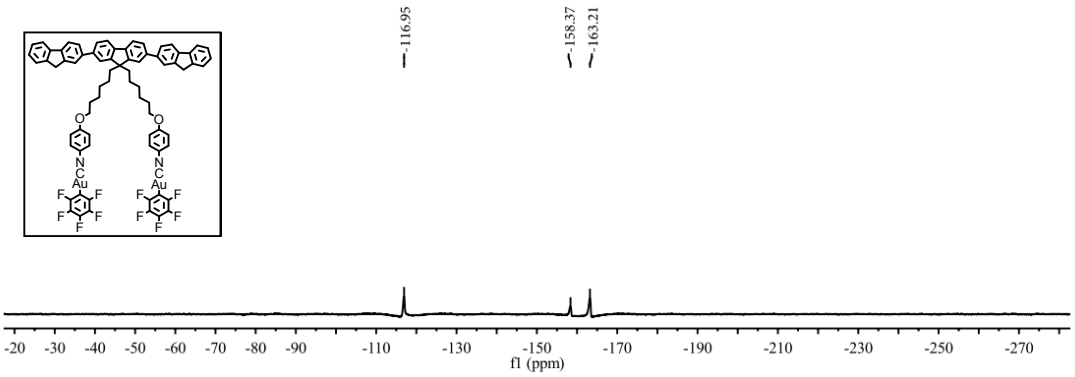
7.68
7.66
7.58
7.57
7.45
7.43
7.41
7.37
7.35
7.33
7.24
7.22
7.20
6.73
6.70
3.94
3.77
3.75
3.74
2.13
1.55
1.26
1.24
1.17
1.15
0.90
0.88
0.86
0.78
0.00
8.99
6.03
2.03
2.03
2.02
3.06
3.99
4.05
4.00
4.07
3.97
8.02
4.05
f1 (ppm)


-116.95
-158.37
-163.21
f1 (ppm)