

Electronic Supplementary Information (ESI)

Carbazole-Based Gold(I) Complexes with Alkyl Chains of Different Lengths: Tunable Solid-State Fluorescence, Aggregation-Induced Emission (AIE), and Reversible Mechanochromism Characteristics

Zhao Chen, Lan Yang, Yuxuan Hu, Di Wu, Jun Yin, Guang-Ao Yu and Sheng Hua Liu**

Key Laboratory of Pesticide and Chemical Biology, Ministry of Education, College of Chemistry, Central China Normal University, Wuhan 430079, P. R. China

Tel: +86-27-67867725 Fax: +86-27-67867725

Corresponding author E-mail: yinj@mail.ccnu.edu.cn; chshliu@mail.ccnu.edu.cn

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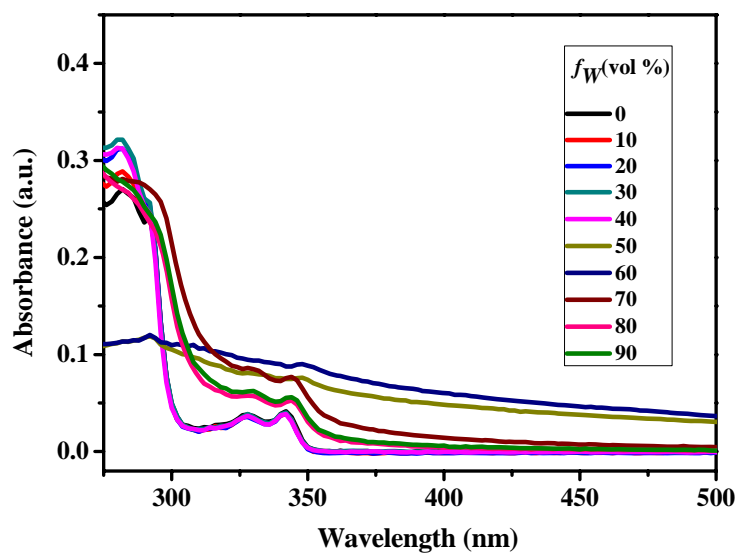


Fig. S1 UV spectra of complex **1** ($1.0 \times 10^{-5} \text{ mol L}^{-1}$) in DMF-water mixtures with various water contents (0-90%).

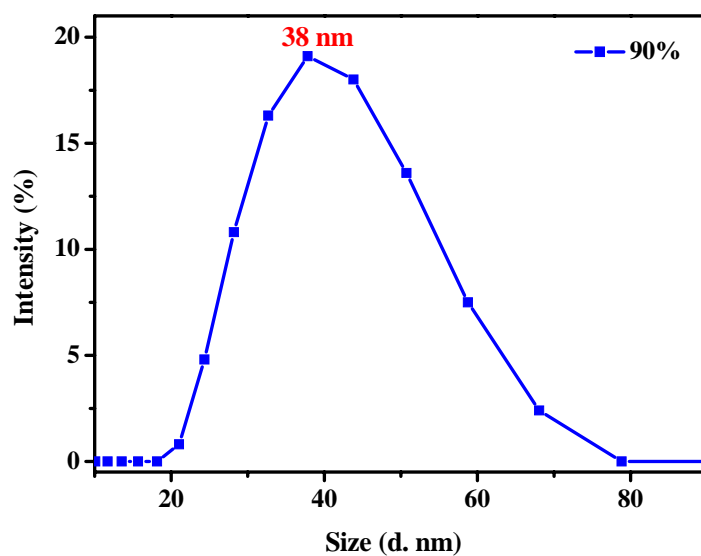


Fig. S2 Size distribution curve of complex **1** ($1.0 \times 10^{-5} \text{ mol L}^{-1}$) in DMF-water mixtures with 90% volume fraction of water.

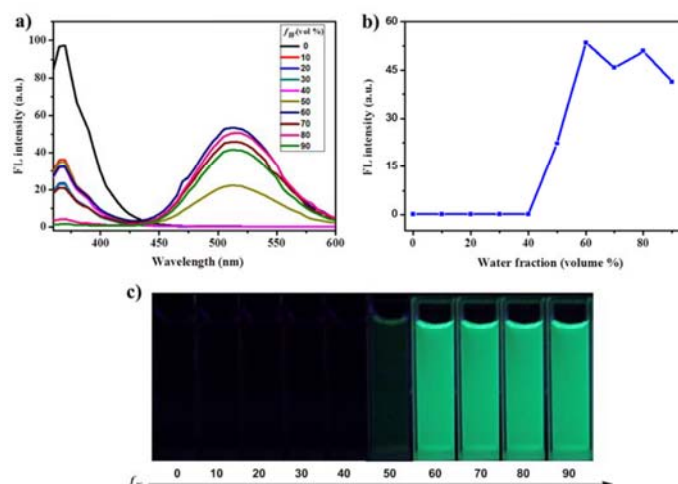


Fig. S3 PL spectra of the dilute solutions of luminogen **2** (1.0×10^{-5} mol L⁻¹) in DMF-H₂O mixtures with different water fractions (f_w). Excitation wavelength = 330 nm. (b) Changes in the emission intensity of **2** at 515 nm in DMF-H₂O mixtures with various volume fractions of water (0-90%). (c) The fluorescence images of **2** (concentration: 1.0×10^{-5} mol L⁻¹) in diverse DMF-H₂O mixtures with various f_w values (0-90%) under 365 nm UV irradiation.

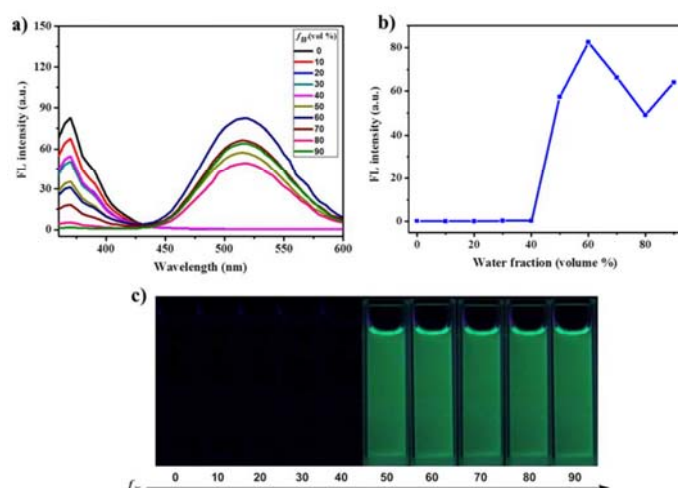


Fig. S4 (a) PL spectra of the dilute solutions of luminogen **3** (1.0×10^{-5} mol L⁻¹) in DMF-H₂O mixtures with different water fractions (f_w). Excitation wavelength = 330 nm. (b) Changes in the emission intensity of **3** at 515 nm in DMF-H₂O mixtures with various volume fractions of water (0-90%). (c) The fluorescence images of **3** (concentration: 1.0×10^{-5} mol L⁻¹) in diverse DMF-H₂O mixtures with various f_w values (0-90%) under 365 nm UV irradiation.

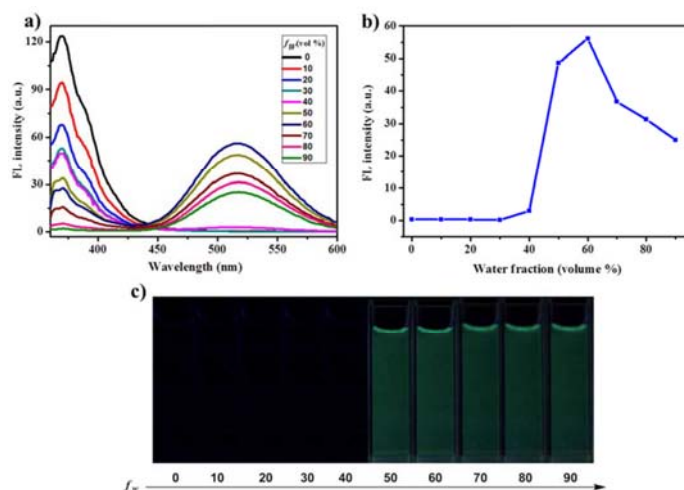


Fig. S5 (a) PL spectra of the dilute solutions of luminogen **4** (1.0×10^{-5} mol L⁻¹) in DMF-H₂O mixtures with different water fractions (f_w). Excitation wavelength = 330 nm. (b) Changes in the emission intensity of **4** at 516 nm in DMF-H₂O mixtures with various volume fractions of water (0-90%). (c) The fluorescence images of **4** (concentration: 1.0×10^{-5} mol L⁻¹) in diverse DMF-H₂O mixtures with various f_w values (0-90%) under 365 nm UV irradiation.

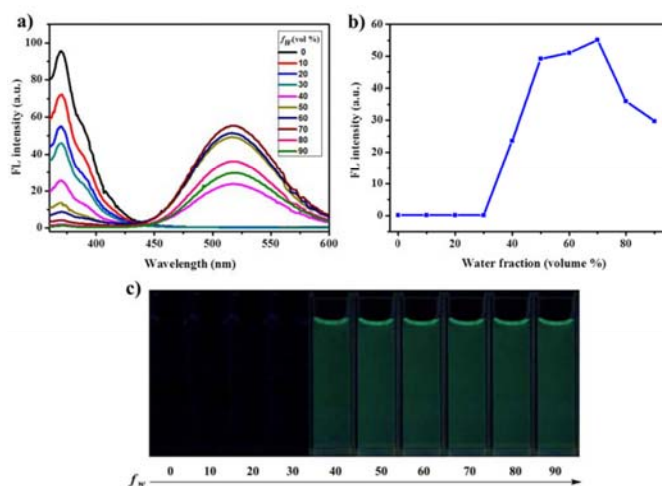


Fig. S6 (a) PL spectra of the dilute solutions of luminogen **5** (1.0×10^{-5} mol L⁻¹) in DMF-H₂O mixtures with different water fractions (f_w). Excitation wavelength = 330 nm. (b) Changes in the emission intensity of **5** at 520 nm in DMF-H₂O mixtures with various volume fractions of water (0-90%). (c) The fluorescence images of **5** (concentration: 1.0×10^{-5} mol L⁻¹) in diverse DMF-H₂O mixtures with various f_w values (0-90%) under 365 nm UV irradiation.

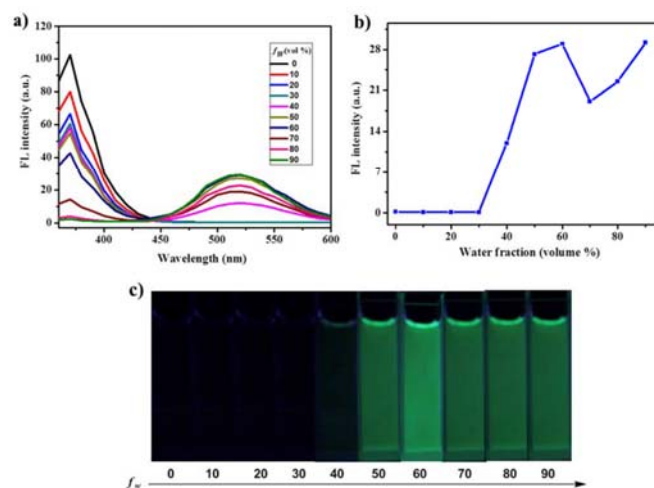


Fig. S7 (a) PL spectra of the dilute solutions of luminogen **6** ($1.0 \times 10^{-5} \text{ mol L}^{-1}$) in DMF-H₂O mixtures with different water fractions (f_w). Excitation wavelength = 330 nm. (b) Changes in the emission intensity of **6** at 520 nm in DMF-H₂O mixtures with various volume fractions of water (0-90%). (c) The fluorescence images of **6** (concentration: $1.0 \times 10^{-5} \text{ mol L}^{-1}$) in diverse DMF-H₂O mixtures with various f_w values (0-90%) under 365 nm UV irradiation.

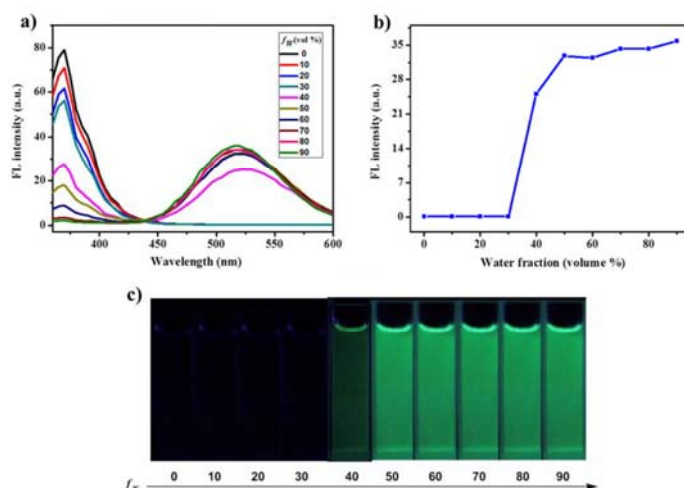


Fig. S8 (a) PL spectra of the dilute solutions of luminogen **7** ($1.0 \times 10^{-5} \text{ mol L}^{-1}$) in DMF-H₂O mixtures with different water fractions (f_w). Excitation wavelength = 330 nm. (b) Changes in the emission intensity of **7** at 520 nm in DMF-H₂O mixtures with various volume fractions of water (0-90%). (c) The fluorescence images of **7** (concentration: $1.0 \times 10^{-5} \text{ mol L}^{-1}$) in diverse DMF-H₂O mixtures with various f_w values (0-90%) under 365 nm UV irradiation.

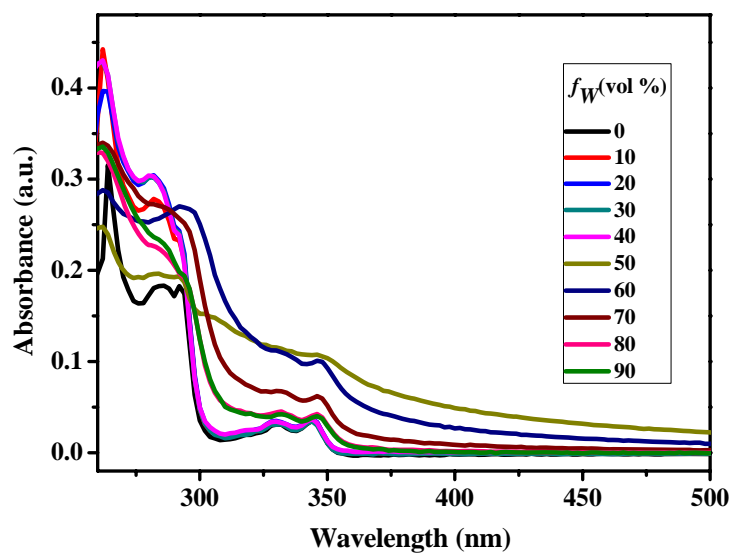


Fig. S9 UV spectra of complex **2** ($1.0 \times 10^{-5} \text{ mol L}^{-1}$) in DMF-water mixtures with various water contents (0-90%).

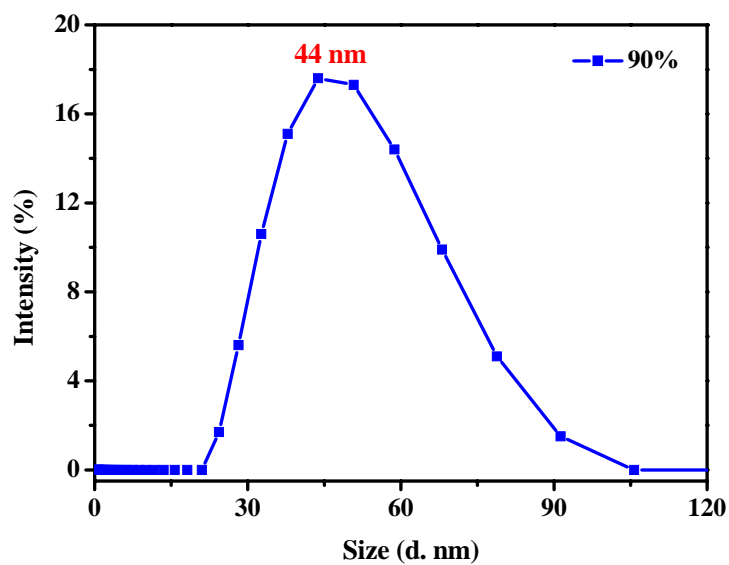


Fig. S10 Size distribution curve of complex **2** ($1.0 \times 10^{-5} \text{ mol L}^{-1}$) in DMF-water mixtures with 90% volume fraction of water.

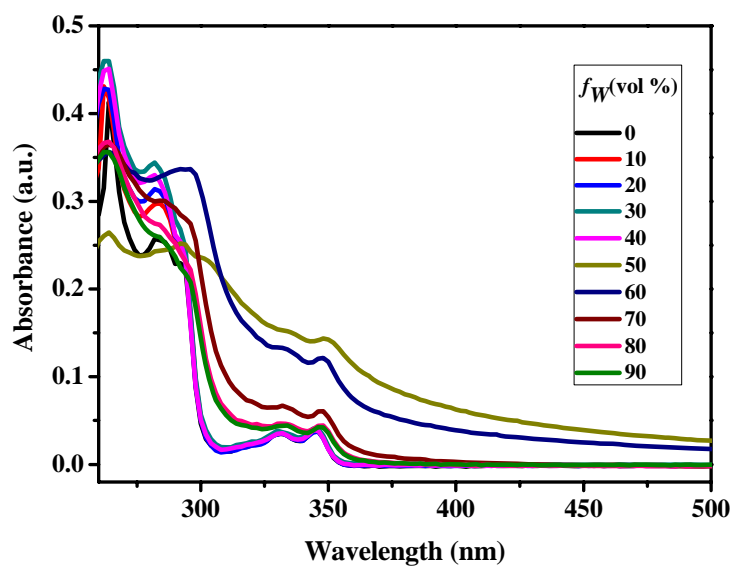


Fig. S11 UV spectra of complex **3** ($1.0 \times 10^{-5} \text{ mol L}^{-1}$) in DMF-water mixtures with various water contents (0-90%).

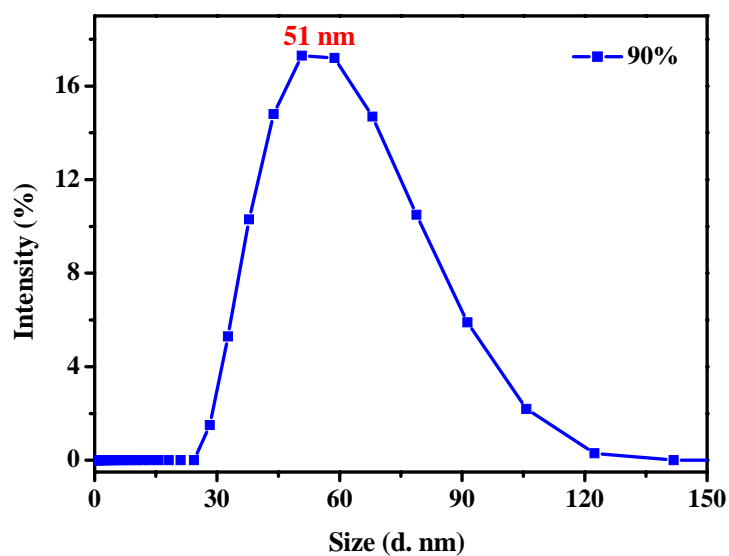


Fig. S12 Size distribution curve of complex **3** ($1.0 \times 10^{-5} \text{ mol L}^{-1}$) in DMF-water mixtures with 90% volume fraction of water.

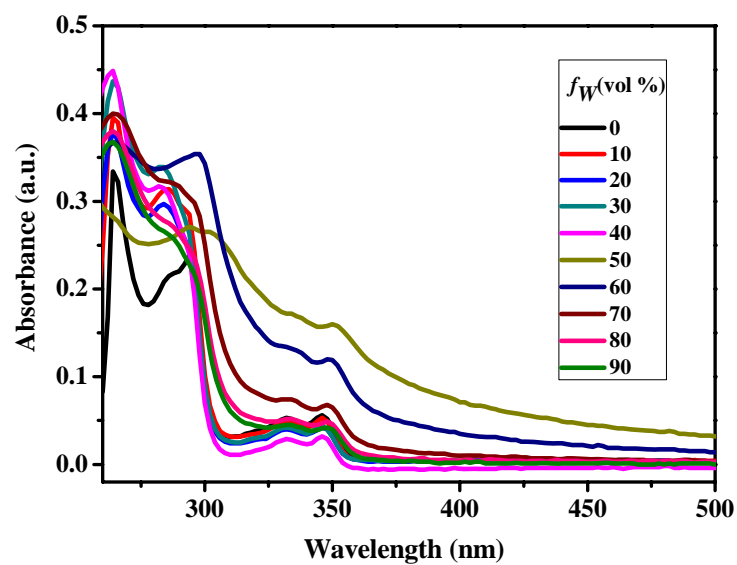


Fig. S13 UV spectra of complex **4** ($1.0 \times 10^{-5} \text{ mol L}^{-1}$) in DMF-water mixtures with various water contents (0-90%).

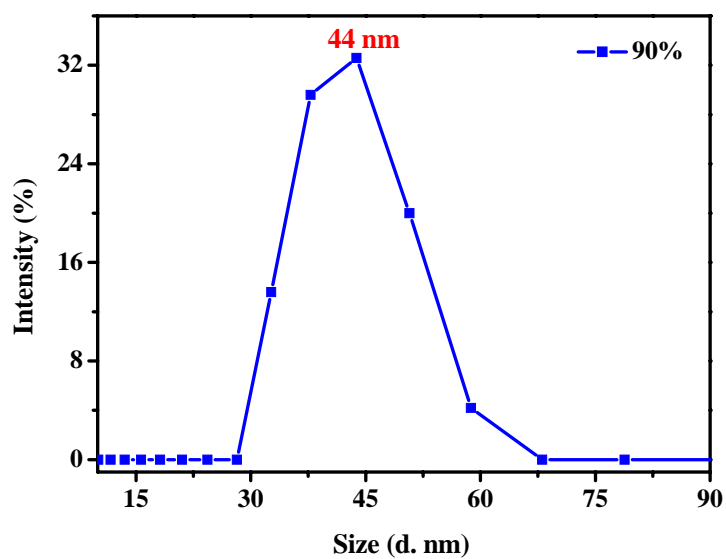


Fig. S14 Size distribution curve of complex **4** ($1.0 \times 10^{-5} \text{ mol L}^{-1}$) in DMF-water mixtures with 90% volume fraction of water.

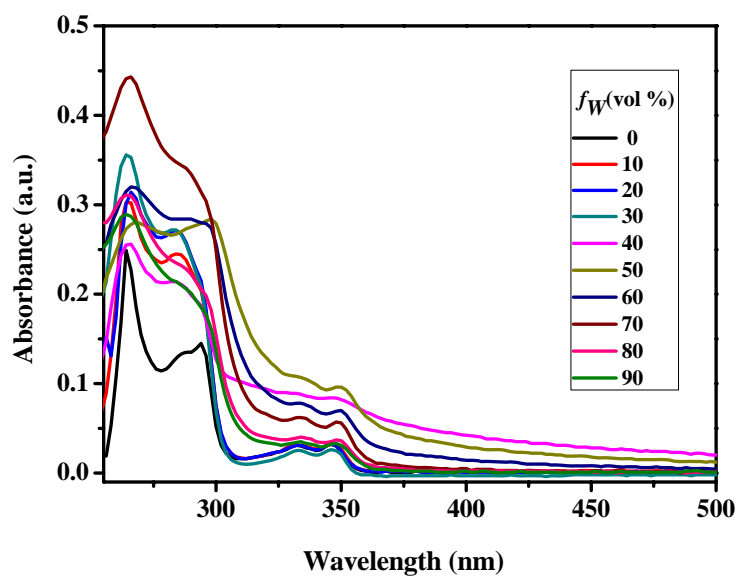


Fig. S15 UV spectra of complex **5** ($1.0 \times 10^{-5} \text{ mol L}^{-1}$) in DMF-water mixtures with various water contents (0-90%).

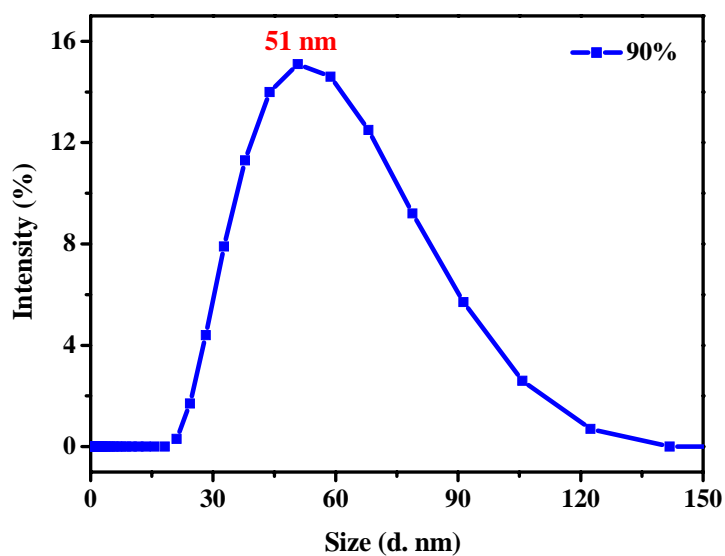


Fig. S16 Size distribution curve of complex **5** ($1.0 \times 10^{-5} \text{ mol L}^{-1}$) in DMF-water mixtures with 90% volume fraction of water.

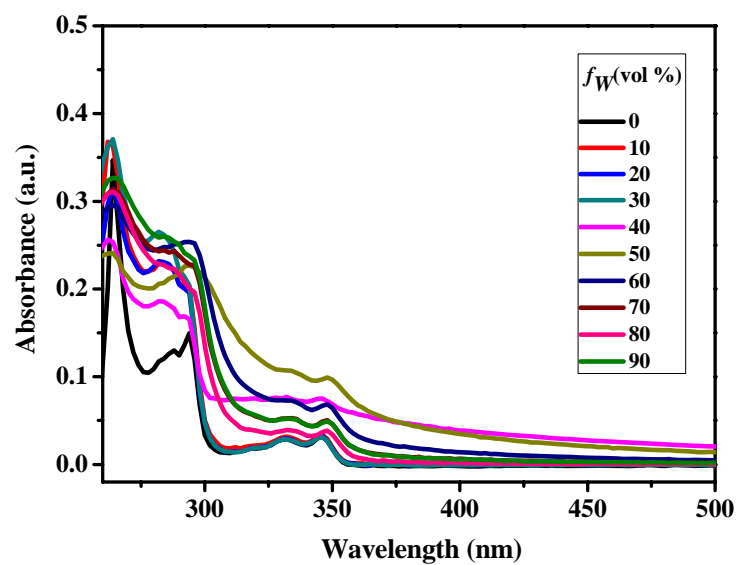


Fig. S17 UV spectra of complex **6** ($1.0 \times 10^{-5} \text{ mol L}^{-1}$) in DMF-water mixtures with various water contents (0-90%).

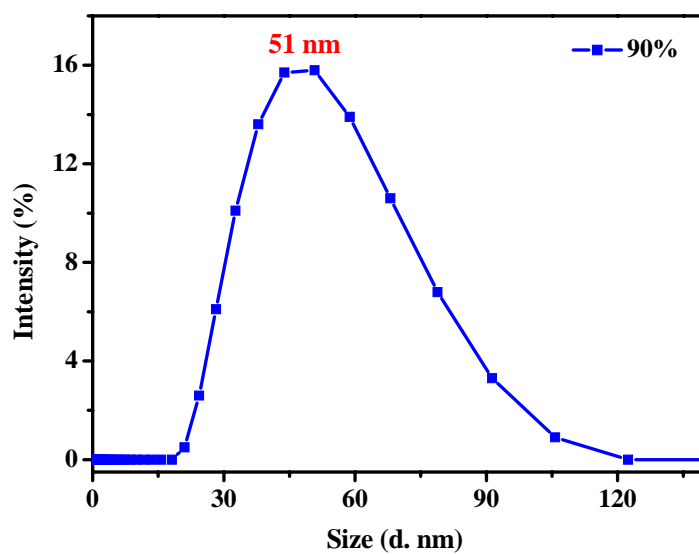


Fig. S18 Size distribution curve of complex **6** ($1.0 \times 10^{-5} \text{ mol L}^{-1}$) in DMF-water mixtures with 90% volume fraction of water.

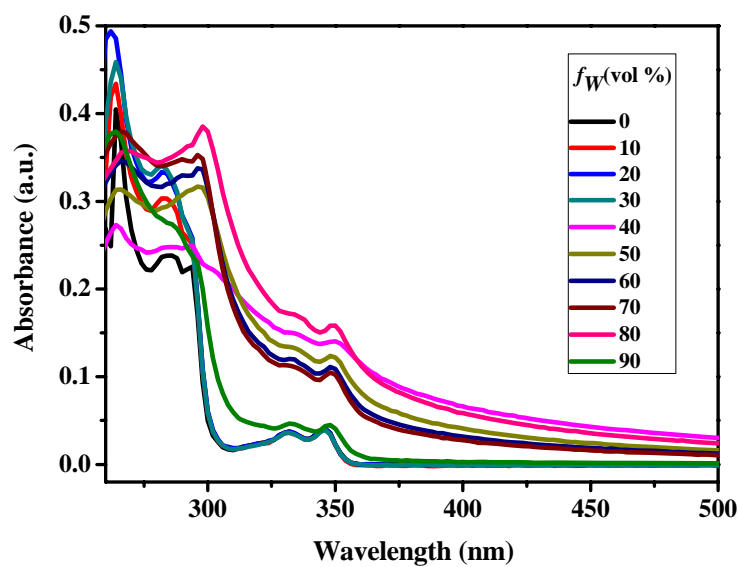


Fig. S19 UV spectra of complex **7** ($1.0 \times 10^{-5} \text{ mol L}^{-1}$) in DMF-water mixtures with various water contents (0-90%).

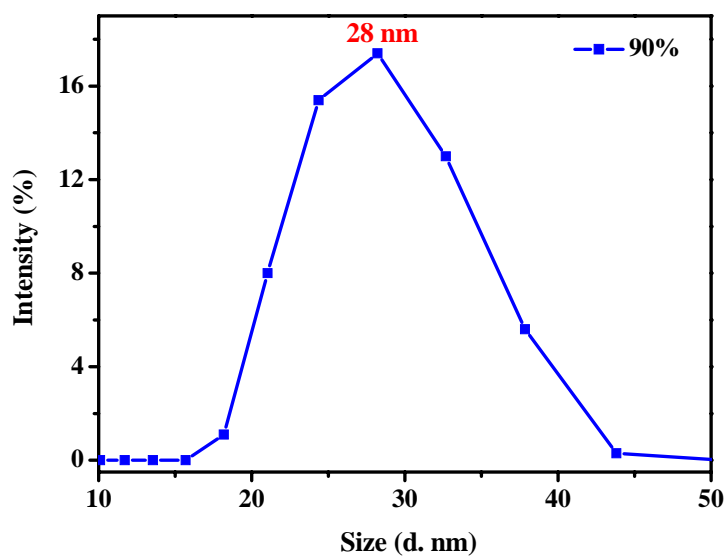


Fig. S20 Size distribution curve of complex **7** ($1.0 \times 10^{-5} \text{ mol L}^{-1}$) in DMF-water mixtures with 90% volume fraction of water.

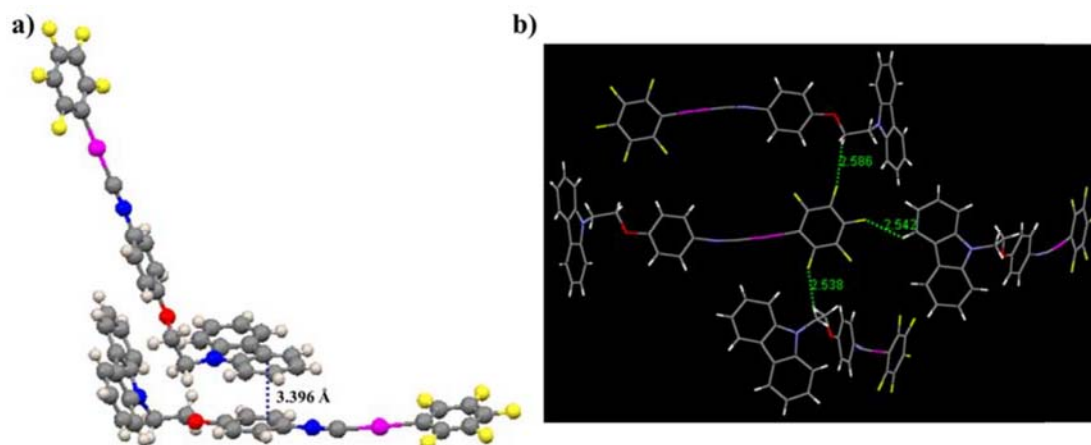


Fig. S21 a) Crystal packing diagram of complex **1**. It showed weak intermolecular $\pi \cdots \pi$ interaction; b) Crystal packing diagram of complex **1**. It showed weak intermolecular C-H \cdots F interactions.

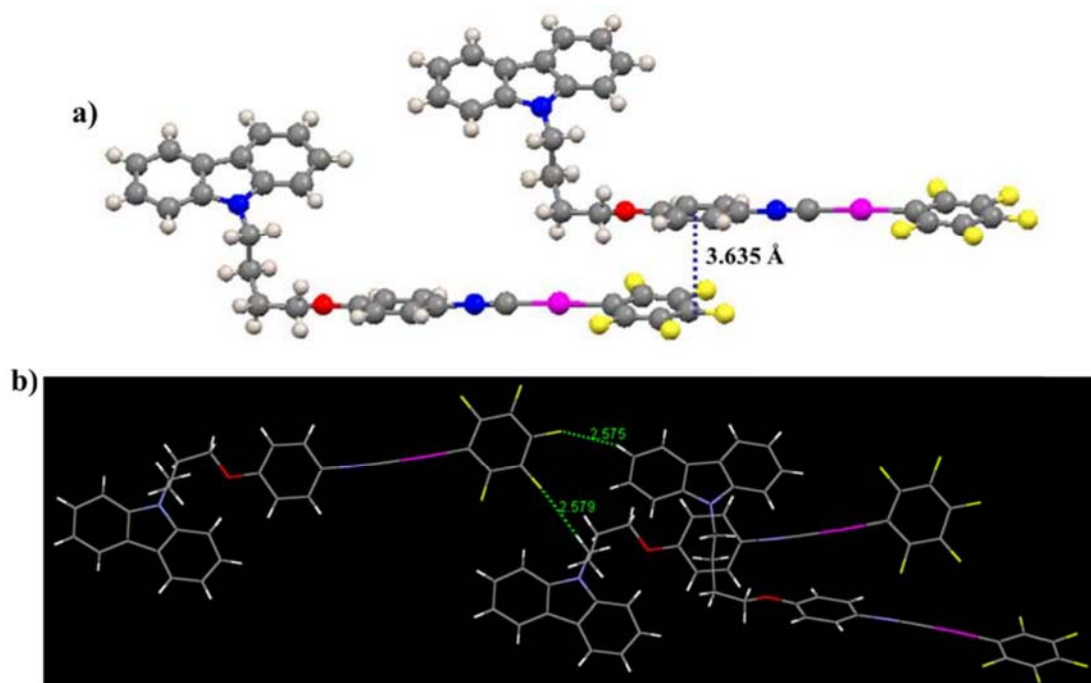


Fig. S22 a) Crystal packing diagram of complex **3**. It showed weak intermolecular $\pi \cdots \pi$ interaction; b) Crystal packing diagram of complex **3**. It showed weak intermolecular C-H \cdots F interactions.

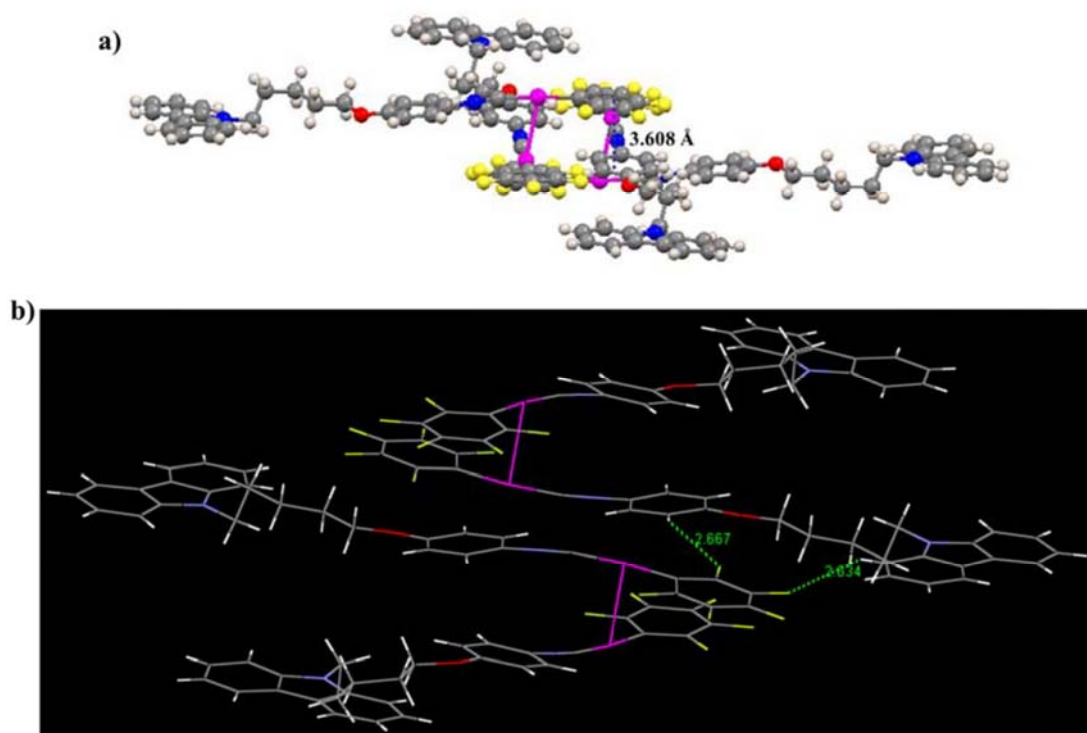


Fig. S23 a) Crystal packing diagram of complex **4**. It showed weak intermolecular $\pi \cdots \pi$ interaction; b) Crystal packing diagram of complex **4**. It showed weak intermolecular C-H \cdots F interactions.

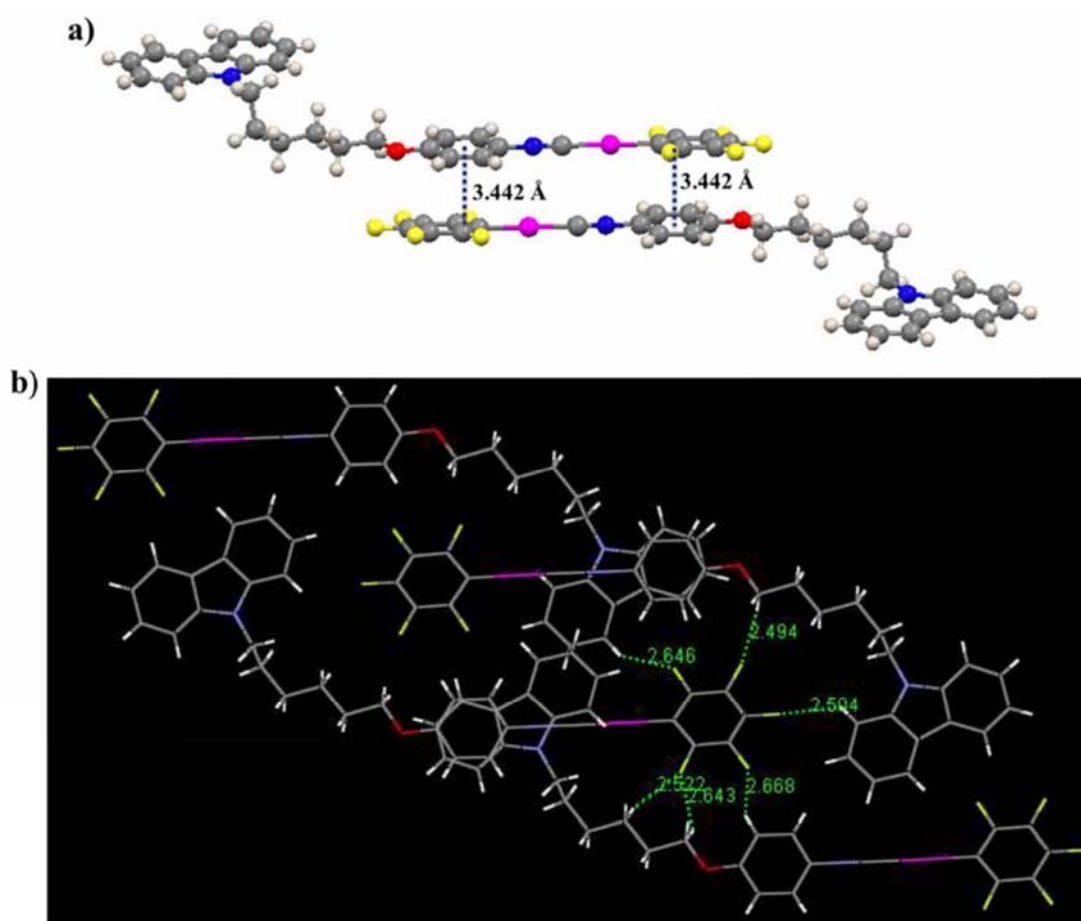


Fig. S24 a) Crystal packing diagram of complex **5**. It showed weak intermolecular $\pi \cdots \pi$ interaction; b) Crystal packing diagram of complex **5**. It showed weak intermolecular C-H \cdots F interactions.

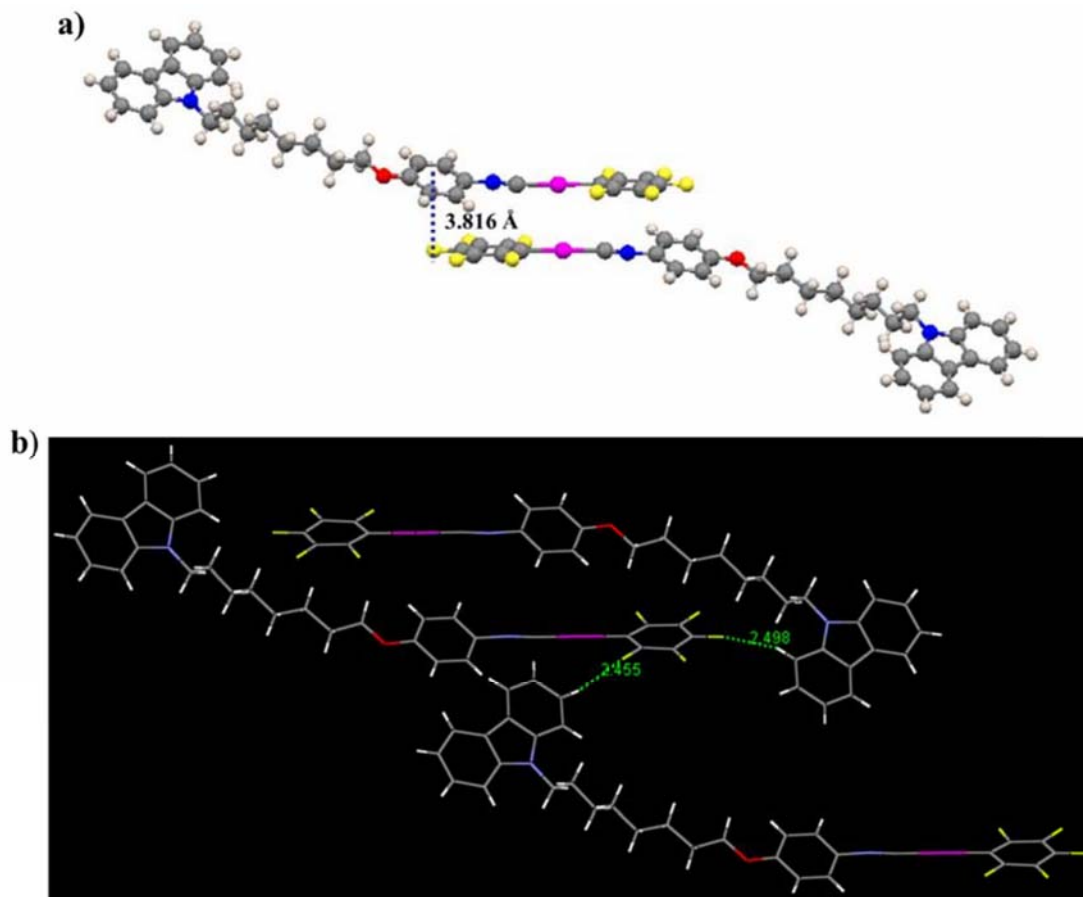


Fig. S25 a) Crystal packing diagram of complex **7**. It showed weak intermolecular $\pi \cdots \pi$ interaction; b) Crystal packing diagram of complex **7**. It showed weak intermolecular C-H \cdots F interactions.

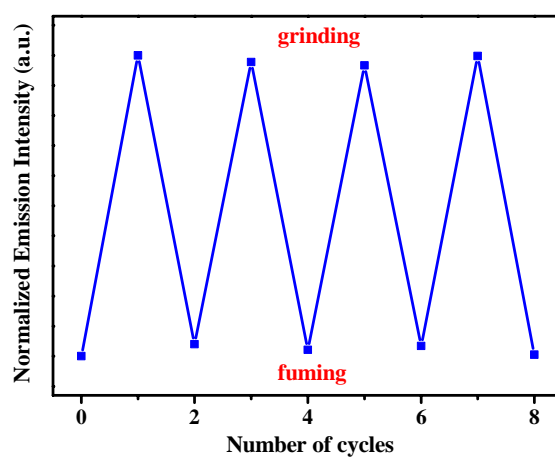


Fig. S26 Invertible grinding-fuming processes of the photoluminescence of complex **1** at 511 nm.

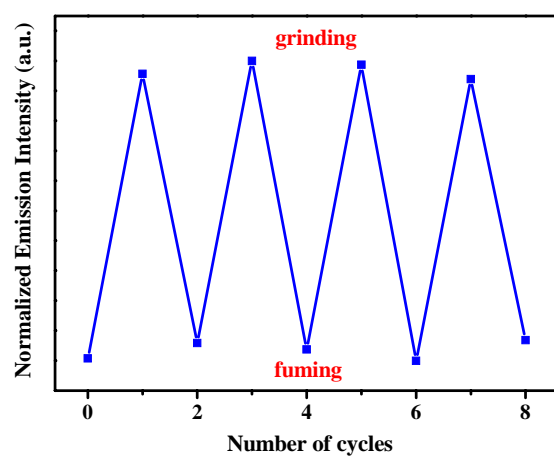


Fig. S27 Invertible grinding-fuming processes of the photoluminescence of complex **2** at 511 nm.

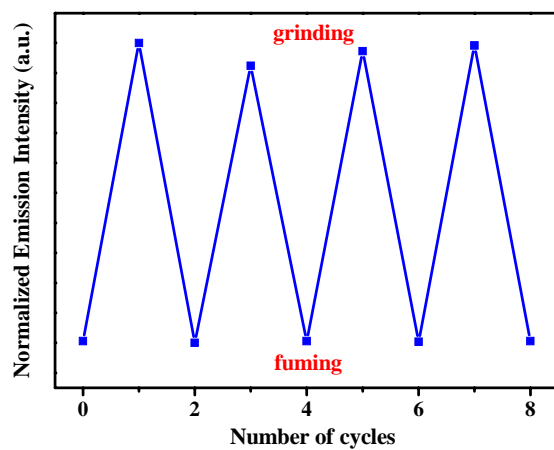


Fig. S28 Invertible grinding-fuming processes of the photoluminescence of complex **3** at 513 nm.

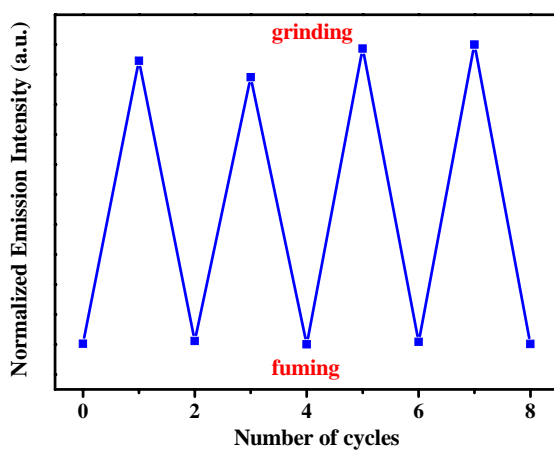


Fig. S29 Invertible grinding-fuming processes of the photoluminescence of complex **4** at 513 nm.

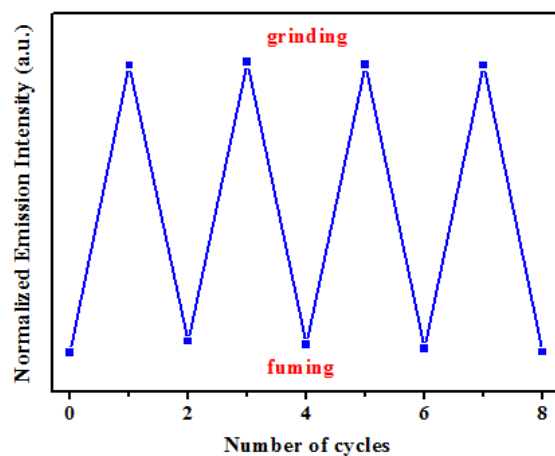


Fig. S30 Invertible grinding-fuming processes of the photoluminescence of complex **5** at 513 nm.

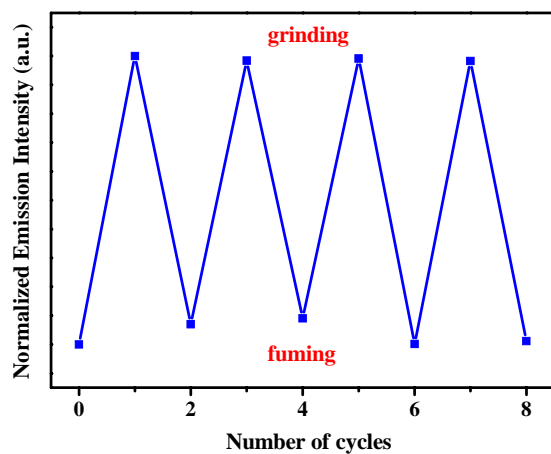


Fig. S31 Invertible grinding-fuming processes of the photoluminescence of complex **6** at 513 nm.

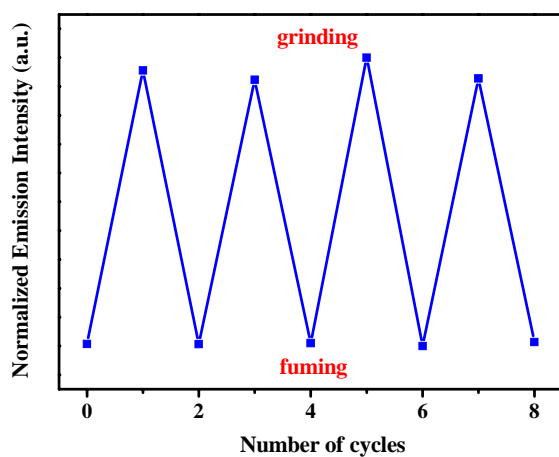


Fig. S32 Invertible grinding-fuming processes of the photoluminescence of complex **7** at 515 nm.

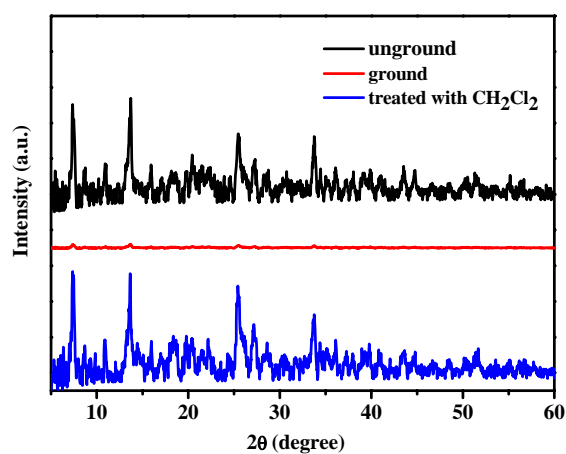


Fig. S33 XRD patterns of complex 2: unground, ground and after treatment with dichloromethane.

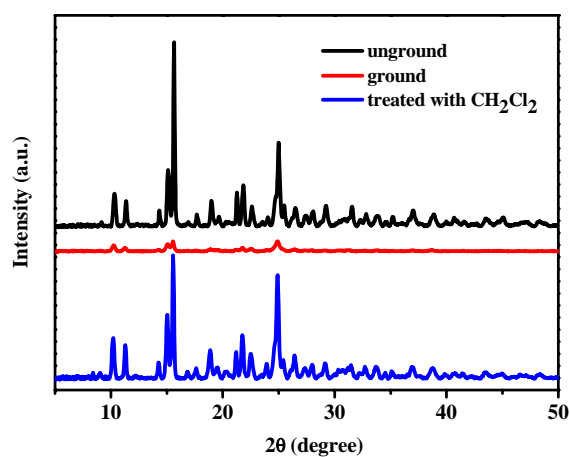


Fig. S34 XRD patterns of complex 3: unground, ground and after treatment with dichloromethane.

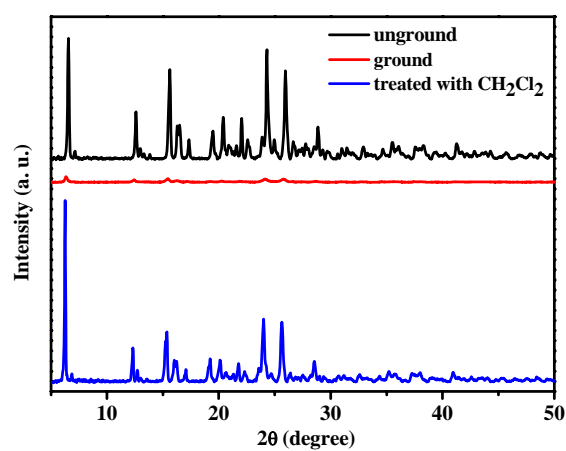


Fig. S35 XRD patterns of complex 5: unground, ground and after treatment with dichloromethane.

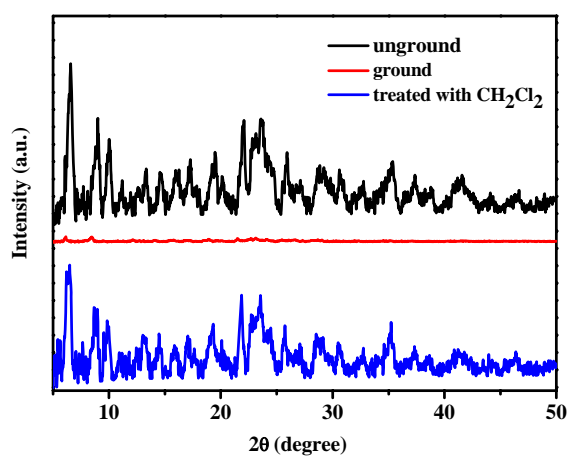


Fig. S36 XRD patterns of complex **6**: unground, ground and after treatment with dichloromethane.

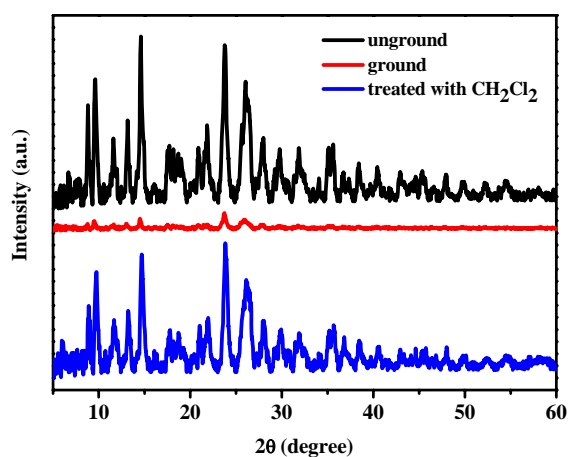


Fig. S37 XRD patterns of complex **7**: unground, ground and after treatment with dichloromethane.

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

Empirical formula	C _{54.50} H ₃₃ Au ₂ Cl F ₁₀ N ₄ O ₂
Formula weight	1395.23
Temperature (K)	298(2)
Crystal system	Monoclinic
Space group	C2/c
<i>a</i> (Å)	28.924(4)
<i>b</i> (Å)	8.5750(11)
<i>c</i> (Å)	40.421(5)
<i>α</i> (deg)	90
<i>β</i> (deg)	102.003(2)

γ (deg)	90
V (\AA^3)	9806(2)
Z	8
Absorption coefficient (mm^{-1})	6.117
F (000)	5352
Theta range for data collection (deg)	1.03 to 25.98
Index ranges	$-34 \leq h \leq 35$, $-10 \leq k \leq 10$, $-49 \leq l \leq 49$
Reflections collected/unique	35964/ 9571 ($R_{\text{int}} = 0.0458$)
Final R indices [$I > 2\sigma(I)$]	$R_1 = 0.0523$, $wR_2 = 0.1456$
R indices (all data)	$R_1 = 0.0870$, $wR_2 = 0.1718$
Goodness-of-fit on F^2	1.050
Largest difference peak and hole (e \AA^{-3})	1.191, -1.070

Table S2. Structure determination summary for the complex **3**.

Empirical formula	$\text{C}_{29} \text{H}_{20} \text{Au F}_5 \text{N}_2 \text{O}$
Formula weight	704.44
Temperature (K)	298(2)
Crystal system	Monoclinic
Space group	$P2(1)/c$
a (\AA)	10.4570(17)
b (\AA)	22.475(4)
c (\AA)	11.8269(19)
α (deg)	90
β (deg)	115.490(2)
γ (deg)	90
V (\AA^3)	2509.1(7)
Z	4
Absorption coefficient (mm^{-1})	5.927
F (000)	1360
Theta range for data collection (deg)	1.81 to 30.83
Index ranges	$-14 \leq h \leq 15$, $-30 \leq k \leq 32$, $-16 \leq l \leq 16$
Reflections collected/unique	25560/ 7797 ($R_{\text{int}} = 0.0461$)
Final R indices [$I > 2\sigma(I)$]	$R_1 = 0.0450$, $wR_2 = 0.1151$

R indices (all data)	$R_1=0.0758$, $wR_2=0.1301$
Goodness-of-fit on F^2	1.019
Largest difference peak and hole($e \text{ \AA}^{-3}$)	1.303, -2.091

Table S3. Structure determination summary for the complex **4**.

Empirical formula	$C_{30} H_{22} Au F_5 N_2 O$
Formula weight	718.46
Temperature (K)	298(2)
Crystal system	Monoclinic
Space group	$C2/c$
a (\AA)	18.208(4)
b (\AA)	17.298(3)
c (\AA)	16.458(3)
α (deg)	90
β (deg)	99.525(3)
γ (deg)	90
V (\AA^3)	5112.1(17)
Z	8
Absorption coefficient (mm^{-1})	5.820
$F(000)$	2784
Theta range for data collection (deg)	1.63 to 25.00
Index ranges	$-21 \leq h \leq 19$, $-20 \leq k \leq 20$, $-19 \leq l \leq 19$
Reflections collected/unique	15327/ 4447 ($R_{\text{int}}=0.0575$)
Final R indices [$I > 2\sigma(I)$]	$R_1=0.0610$, $wR_2=0.1675$
R indices (all data)	$R_1=0.0809$, $wR_2=0.1871$
Goodness-of-fit on F^2	1.051
Largest difference peak and hole($e \text{ \AA}^{-3}$)	2.111, -1.248

Table S4. Structure determination summary for the complex **5**.

Empirical formula	$C_{31} H_{24} Au F_5 N_2 O$
Formula weight	732.49
Temperature (K)	295(2)

Crystal system	Triclinic
Space group	P-1
<i>a</i> (Å)	7.6240(11)
<i>b</i> (Å)	13.6244(18)
<i>c</i> (Å)	14.516(2)
α (deg)	102.723(2)
β (deg)	100.056(2)
γ (deg)	105.814(2)
<i>V</i> (Å ³)	1370.2(3)
Z	2
Absorption coefficient (mm ⁻¹)	5.430
F (000)	712
Theta range for data collection (deg)	1.49 to 26.00
Index ranges	-9<= <i>h</i> <=9, -16<= <i>k</i> <=16, -17<= <i>l</i> <=17
Reflections collected/unique	10466/5355 (<i>R</i> _{int} = 0.0328)
Final R indices [<i>I</i> >2σ(<i>I</i>)]	<i>R</i> ₁ = 0.0366, <i>wR</i> ₂ = 0.1131
R indices (all data)	<i>R</i> ₁ = 0.0414, <i>wR</i> ₂ = 0.1207
Goodness-of-fit on <i>F</i> ²	1.103
Largest difference peak and hole(e Å ⁻³)	0.851, -1.692

Table S5. Structure determination summary for the complex **7**.

Empirical formula	C ₃₃ H ₂₈ Au F ₅ N ₂ O
Formula weight	760.54
Temperature (K)	273(2)
Crystal system	Monoclinic
Space group	C2/c
<i>a</i> (Å)	19.127(3)
<i>b</i> (Å)	7.5247(11)
<i>c</i> (Å)	41.685(7)
α (deg)	90
β (deg)	101.562(2)
γ (deg)	90
<i>V</i> (Å ³)	5877.8(15)
Z	8
Absorption coefficient (mm ⁻¹)	5.067

F (000)	2976
Theta range for data collection (deg)	2.17 to 26.00
Index ranges	-23<=h<=22, -9<=k<=9, -51<=l<=51
Reflections collected/unique	19498/ 5747 (R _{int} = 0.0831)
Final R indices [I>2sigma(I)]	R ₁ = 0.0928, wR ₂ = 0.2082
R indices (all data)	R ₁ = 0.1197, wR ₂ = 0.2232
Goodness-of-fit on F ²	1.184
Largest difference peak and hole(e Å ⁻³)	1.519, -2.178

Table S6. Bond lengths [Å] and angles [°] of **1**.

Au(1)-C(7)	1.948(11)	C(11)-O(1)	1.395(11)
Au(1)-C(1)	2.038(9)	C(12)-C(13)	1.359(14)
Au(1)-Au(2)	3.4073(7)	C(12)-H(12)	0.9300
Au(2)-C(34)	1.942(11)	C(13)-H(13)	0.9300
Au(2)-C(28)	1.997(10)	C(14)-O(1)	1.400(11)
C(1)-C(3)	1.371(13)	C(14)-C(15)	1.491(14)
C(1)-C(2)	1.374(15)	C(14)-H(14A)	0.9700
C(2)-F(5)	1.317(13)	C(14)-H(14B)	0.9700
C(2)-C(6)	1.410(17)	C(15)-N(2)	1.477(12)
C(3)-C(4)	1.347(15)	C(15)-H(15A)	0.9700
C(3)-F(1)	1.369(12)	C(15)-H(15B)	0.9700
C(4)-C(5)	1.314(16)	C(16)-N(2)	1.366(12)
C(4)-F(2)	1.388(12)	C(16)-C(17)	1.409(13)
C(5)-C(6)	1.338(17)	C(16)-C(21)	1.413(13)
C(5)-F(3)	1.348(12)	C(17)-C(18)	1.369(18)
C(6)-F(4)	1.333(13)	C(17)-H(17)	0.9300
C(7)-N(1)	1.162(13)	C(18)-C(19)	1.35(2)
C(8)-C(9)	1.369(16)	C(18)-H(18)	0.9300
C(8)-C(13)	1.412(16)	C(19)-C(20)	1.401(18)
C(8)-N(1)	1.418(13)	C(19)-H(19)	0.9300
C(9)-C(10)	1.357(15)	C(20)-C(21)	1.400(15)
C(9)-H(9)	0.9300	C(20)-H(20)	0.9300
C(10)-C(11)	1.391(14)	C(21)-C(22)	1.448(14)
C(10)-H(10)	0.9300	C(22)-C(23)	1.374(15)
C(11)-C(12)	1.352(14)	C(22)-C(27)	1.383(14)

C(23)-C(24)	1.37(2)	C(42)-H(42A)	0.9700
C(23)-H(23)	0.9300	C(42)-H(42B)	0.9700
C(24)-C(25)	1.37(2)	C(43)-N(4)	1.380(11)
C(24)-H(24)	0.9300	C(43)-C(44)	1.385(16)
C(25)-C(26)	1.449(19)	C(43)-C(48)	1.391(14)
C(25)-H(25)	0.9300	C(44)-C(45)	1.431(15)
C(26)-C(27)	1.392(14)	C(44)-H(44)	0.9300
C(26)-H(26)	0.9300	C(45)-C(46)	1.388(18)
C(27)-N(2)	1.383(10)	C(45)-H(45)	0.9300
C(28)-C(33)	1.358(16)	C(46)-C(47)	1.37(2)
C(28)-C(29)	1.397(17)	C(46)-H(46)	0.9300
C(29)-F(6)	1.348(15)	C(47)-C(48)	1.387(15)
C(29)-C(30)	1.412(16)	C(47)-H(47)	0.9300
C(30)-F(7)	1.311(16)	C(48)-C(49)	1.447(16)
C(30)-C(31)	1.41(2)	C(49)-C(54)	1.377(14)
C(31)-C(32)	1.33(2)	C(49)-C(50)	1.398(17)
C(31)-F(8)	1.354(14)	C(50)-C(51)	1.42(2)
C(32)-C(33)	1.354(18)	C(50)-H(50)	0.9300
C(32)-F(9)	1.363(15)	C(51)-C(52)	1.38(2)
C(33)-F(10)	1.384(16)	C(51)-H(51)	0.9300
C(34)-N(3)	1.186(12)	C(52)-C(53)	1.387(17)
C(35)-C(40)	1.350(13)	C(52)-H(52)	0.9300
C(35)-N(3)	1.372(13)	C(53)-C(54)	1.383(14)
C(35)-C(36)	1.383(14)	C(53)-H(53)	0.9300
C(36)-C(37)	1.376(14)	C(54)-N(4)	1.408(12)
C(36)-H(36)	0.9300	C(55)-Cl(1)#1	1.698(10)
C(37)-C(38)	1.362(13)	C(55)-Cl(1)	1.747(10)
C(37)-H(37)	0.9300	C(55)-H(55A)	0.9700
C(38)-O(2)	1.348(11)	C(55)-H(55B)	0.9700
C(38)-C(39)	1.370(12)	Cl(1)-C(55)#1	1.698(10)
C(39)-C(40)	1.393(12)	C(7)-Au(1)-C(1)	176.0(4)
C(39)-H(39)	0.9300	C(7)-Au(1)-Au(2)	100.9(3)
C(40)-H(40)	0.9300	C(1)-Au(1)-Au(2)	80.8(2)
C(41)-O(2)	1.415(10)	C(34)-Au(2)-C(28)	177.1(4)
C(41)-C(42)	1.490(13)	C(34)-Au(2)-Au(1)	97.0(3)
C(41)-H(41A)	0.9700	C(28)-Au(2)-Au(1)	85.1(3)
C(41)-H(41B)	0.9700	C(3)-C(1)-C(2)	114.8(9)
C(42)-N(4)	1.471(10)	C(3)-C(1)-Au(1)	124.0(7)

C(2)-C(1)-Au(1)	121.1(8)	O(1)-C(14)-H(14B)	110.2
F(5)-C(2)-C(1)	120.4(10)	C(15)-C(14)-H(14B)	110.2
F(5)-C(2)-C(6)	117.7(11)	H(14A)-C(14)-H(14B)	108.5
C(1)-C(2)-C(6)	121.9(11)	N(2)-C(15)-C(14)	113.2(8)
C(4)-C(3)-F(1)	118.1(10)	N(2)-C(15)-H(15A)	108.9
C(4)-C(3)-C(1)	123.3(10)	C(14)-C(15)-H(15A)	108.9
F(1)-C(3)-C(1)	118.5(9)	N(2)-C(15)-H(15B)	108.9
C(5)-C(4)-C(3)	120.3(10)	C(14)-C(15)-H(15B)	108.9
C(5)-C(4)-F(2)	119.8(10)	H(15A)-C(15)-H(15B)	107.8
C(3)-C(4)-F(2)	119.8(11)	N(2)-C(16)-C(17)	128.5(9)
C(4)-C(5)-C(6)	121.5(11)	N(2)-C(16)-C(21)	107.9(8)
C(4)-C(5)-F(3)	119.9(12)	C(17)-C(16)-C(21)	123.5(10)
C(6)-C(5)-F(3)	118.5(13)	C(18)-C(17)-C(16)	115.7(12)
F(4)-C(6)-C(5)	124.4(12)	C(18)-C(17)-H(17)	122.1
F(4)-C(6)-C(2)	117.5(12)	C(16)-C(17)-H(17)	122.1
C(5)-C(6)-C(2)	118.0(11)	C(19)-C(18)-C(17)	123.3(13)
N(1)-C(7)-Au(1)	173.1(10)	C(19)-C(18)-H(18)	118.4
C(9)-C(8)-C(13)	120.9(10)	C(17)-C(18)-H(18)	118.4
C(9)-C(8)-N(1)	120.4(11)	C(18)-C(19)-C(20)	121.2(12)
C(13)-C(8)-N(1)	118.7(11)	C(18)-C(19)-H(19)	119.4
C(10)-C(9)-C(8)	119.9(11)	C(20)-C(19)-H(19)	119.4
C(10)-C(9)-H(9)	120.0	C(19)-C(20)-C(21)	119.1(11)
C(8)-C(9)-H(9)	120.0	C(19)-C(20)-H(20)	120.5
C(9)-C(10)-C(11)	119.3(11)	C(21)-C(20)-H(20)	120.5
C(9)-C(10)-H(10)	120.3	C(20)-C(21)-C(16)	117.2(11)
C(11)-C(10)-H(10)	120.3	C(20)-C(21)-C(22)	135.9(10)
C(12)-C(11)-C(10)	120.6(9)	C(16)-C(21)-C(22)	106.9(8)
C(12)-C(11)-O(1)	115.2(9)	C(23)-C(22)-C(27)	121.1(11)
C(10)-C(11)-O(1)	124.2(10)	C(23)-C(22)-C(21)	132.6(11)
C(11)-C(12)-C(13)	121.6(11)	C(27)-C(22)-C(21)	106.3(8)
C(11)-C(12)-H(12)	119.2	C(24)-C(23)-C(22)	117.8(13)
C(13)-C(12)-H(12)	119.2	C(24)-C(23)-H(23)	121.1
C(12)-C(13)-C(8)	117.5(11)	C(22)-C(23)-H(23)	121.1
C(12)-C(13)-H(13)	121.2	C(25)-C(24)-C(23)	121.9(14)
C(8)-C(13)-H(13)	121.2	C(25)-C(24)-H(24)	119.1
O(1)-C(14)-C(15)	107.5(8)	C(23)-C(24)-H(24)	119.0
O(1)-C(14)-H(14A)	110.2	C(24)-C(25)-C(26)	122.1(14)
C(15)-C(14)-H(14A)	110.2	C(24)-C(25)-H(25)	119.0

C(26)-C(25)-H(25)	119.0	C(38)-C(39)-C(40)	120.0(8)
C(27)-C(26)-C(25)	113.3(12)	C(38)-C(39)-H(39)	120.0
C(27)-C(26)-H(26)	123.3	C(40)-C(39)-H(39)	120.0
C(25)-C(26)-H(26)	123.3	C(35)-C(40)-C(39)	120.2(9)
N(2)-C(27)-C(22)	109.3(8)	C(35)-C(40)-H(40)	119.9
N(2)-C(27)-C(26)	127.1(10)	C(39)-C(40)-H(40)	119.9
C(22)-C(27)-C(26)	123.6(9)	O(2)-C(41)-C(42)	107.7(8)
C(33)-C(28)-C(29)	112.6(11)	O(2)-C(41)-H(41A)	110.2
C(33)-C(28)-Au(2)	126.8(10)	C(42)-C(41)-H(41A)	110.2
C(29)-C(28)-Au(2)	120.6(9)	O(2)-C(41)-H(41B)	110.2
F(6)-C(29)-C(28)	121.5(10)	C(42)-C(41)-H(41B)	110.2
F(6)-C(29)-C(30)	113.1(13)	H(41A)-C(41)-H(41B)	108.5
C(28)-C(29)-C(30)	125.4(13)	N(4)-C(42)-C(41)	113.3(7)
F(7)-C(30)-C(31)	122.3(13)	N(4)-C(42)-H(42A)	108.9
F(7)-C(30)-C(29)	122.6(13)	C(41)-C(42)-H(42A)	108.9
C(31)-C(30)-C(29)	115.0(14)	N(4)-C(42)-H(42B)	108.9
C(32)-C(31)-F(8)	121.7(17)	C(41)-C(42)-H(42B)	108.9
C(32)-C(31)-C(30)	120.9(11)	H(42A)-C(42)-H(42B)	107.7
F(8)-C(31)-C(30)	117.4(18)	N(4)-C(43)-C(44)	126.9(9)
C(31)-C(32)-C(33)	120.5(14)	N(4)-C(43)-C(48)	110.3(9)
C(31)-C(32)-F(9)	117.4(14)	C(44)-C(43)-C(48)	122.8(10)
C(33)-C(32)-F(9)	122.1(16)	C(43)-C(44)-C(45)	117.4(12)
C(32)-C(33)-C(28)	125.6(15)	C(43)-C(44)-H(44)	121.3
C(32)-C(33)-F(10)	116.7(13)	C(45)-C(44)-H(44)	121.3
C(28)-C(33)-F(10)	117.7(11)	C(46)-C(45)-C(44)	118.6(13)
N(3)-C(34)-Au(2)	177.3(9)	C(46)-C(45)-H(45)	120.7
C(40)-C(35)-N(3)	121.4(9)	C(44)-C(45)-H(45)	120.7
C(40)-C(35)-C(36)	120.2(9)	C(47)-C(46)-C(45)	122.6(11)
N(3)-C(35)-C(36)	118.4(9)	C(47)-C(46)-H(46)	118.7
C(37)-C(36)-C(35)	118.9(9)	C(45)-C(46)-H(46)	118.7
C(37)-C(36)-H(36)	120.5	C(46)-C(47)-C(48)	119.4(12)
C(35)-C(36)-H(36)	120.5	C(46)-C(47)-H(47)	120.3
C(38)-C(37)-C(36)	121.6(9)	C(48)-C(47)-H(47)	120.3
C(38)-C(37)-H(37)	119.2	C(47)-C(48)-C(43)	119.0(12)
C(36)-C(37)-H(37)	119.2	C(47)-C(48)-C(49)	134.8(11)
O(2)-C(38)-C(37)	116.1(8)	C(43)-C(48)-C(49)	106.2(9)
O(2)-C(38)-C(39)	124.9(8)	C(54)-C(49)-C(50)	119.6(13)
C(37)-C(38)-C(39)	119.0(9)	C(54)-C(49)-C(48)	107.0(9)

C(50)-C(49)-C(48)	133.3(13)	Cl(1)#1-C(55)-H(55A)	112.6
C(49)-C(50)-C(51)	117.3(16)	Cl(1)-C(55)-H(55A)	112.6
C(49)-C(50)-H(50)	121.4	Cl(1)#1-C(55)-H(55B)	112.6
C(51)-C(50)-H(50)	121.4	Cl(1)-C(55)-H(55B)	112.6
C(52)-C(51)-C(50)	121.3(15)	H(55A)-C(55)-H(55B)	110.1
C(52)-C(51)-H(51)	119.3	C(55)#1-Cl(1)-C(55)	84.3(10)
C(50)-C(51)-H(51)	119.3	C(7)-N(1)-C(8)	170.9(13)
C(51)-C(52)-C(53)	121.1(15)	C(16)-N(2)-C(27)	109.6(8)
C(51)-C(52)-H(52)	119.4	C(16)-N(2)-C(15)	123.9(8)
C(53)-C(52)-H(52)	119.4	C(27)-N(2)-C(15)	126.5(8)
C(54)-C(53)-C(52)	116.9(13)	C(34)-N(3)-C(35)	175.3(10)
C(54)-C(53)-H(53)	121.6	C(43)-N(4)-C(54)	106.8(7)
C(52)-C(53)-H(53)	121.6	C(43)-N(4)-C(42)	125.5(9)
C(49)-C(54)-C(53)	123.7(10)	C(54)-N(4)-C(42)	127.8(8)
C(49)-C(54)-N(4)	109.7(9)	C(11)-O(1)-C(14)	117.8(7)
C(53)-C(54)-N(4)	126.6(9)	C(38)-O(2)-C(41)	119.8(7)
Cl(1)#1-C(55)-Cl(1)	95.7(10)		

Table S7. Bond lengths [\AA] and angles [$^\circ$] of **3**.

Au(1)-C(7)	1.961(6)	C(9)-H(9)	0.9300
Au(1)-C(1)	2.028(5)	C(10)-C(11)	1.393(6)
C(1)-C(2)	1.385(7)	C(10)-H(10)	0.9300
C(1)-C(6)	1.400(7)	C(11)-O(1)	1.348(5)
C(2)-C(3)	1.340(7)	C(11)-C(12)	1.398(6)
C(2)-F(1)	1.354(5)	C(12)-C(13)	1.379(6)
C(3)-F(2)	1.351(6)	C(12)-H(12)	0.9300
C(3)-C(4)	1.367(7)	C(13)-H(13)	0.9300
C(4)-F(3)	1.348(6)	C(14)-O(1)	1.444(6)
C(4)-C(5)	1.377(8)	C(14)-C(15)	1.492(7)
C(5)-F(4)	1.344(6)	C(14)-H(14A)	0.9700
C(5)-C(6)	1.359(8)	C(14)-H(14B)	0.9700
C(6)-F(5)	1.355(6)	C(15)-C(16)	1.528(7)
C(7)-N(1)	1.151(7)	C(15)-H(15A)	0.9700
C(8)-C(13)	1.375(7)	C(15)-H(15B)	0.9700
C(8)-C(9)	1.375(7)	C(16)-C(17)	1.512(7)
C(8)-N(1)	1.408(6)	C(16)-H(16A)	0.9700
C(9)-C(10)	1.371(7)	C(16)-H(16B)	0.9700

C(17)-N(2)	1.461(5)	C(3)-C(4)-C(5)	118.8(5)
C(17)-H(17A)	0.9700	F(4)-C(5)-C(6)	121.2(5)
C(17)-H(17B)	0.9700	F(4)-C(5)-C(4)	119.3(5)
C(18)-N(2)	1.386(6)	C(6)-C(5)-C(4)	119.4(5)
C(18)-C(26)	1.397(7)	F(5)-C(6)-C(5)	117.2(4)
C(18)-C(19)	1.403(6)	F(5)-C(6)-C(1)	119.1(5)
C(19)-C(29)	1.397(6)	C(5)-C(6)-C(1)	123.7(5)
C(19)-C(20)	1.441(6)	N(1)-C(7)-Au(1)	178.5(5)
C(20)-C(25)	1.381(6)	C(13)-C(8)-C(9)	121.0(4)
C(20)-C(21)	1.403(7)	C(13)-C(8)-N(1)	120.2(4)
C(21)-N(2)	1.388(6)	C(9)-C(8)-N(1)	118.7(4)
C(21)-C(22)	1.389(6)	C(10)-C(9)-C(8)	120.3(4)
C(22)-C(23)	1.392(8)	C(10)-C(9)-H(9)	119.9
C(22)-H(22)	0.9300	C(8)-C(9)-H(9)	119.9
C(23)-C(24)	1.375(11)	C(9)-C(10)-C(11)	119.8(4)
C(23)-H(23)	0.9300	C(9)-C(10)-H(10)	120.1
C(24)-C(25)	1.370(8)	C(11)-C(10)-H(10)	120.1
C(24)-H(24)	0.9300	O(1)-C(11)-C(10)	124.7(4)
C(25)-H(25)	0.9300	O(1)-C(11)-C(12)	116.1(4)
C(26)-C(27)	1.385(8)	C(10)-C(11)-C(12)	119.3(4)
C(26)-H(26)	0.9300	C(13)-C(12)-C(11)	120.3(4)
C(27)-C(28)	1.386(9)	C(13)-C(12)-H(12)	119.9
C(27)-H(27)	0.9300	C(11)-C(12)-H(12)	119.9
C(28)-C(29)	1.360(8)	C(8)-C(13)-C(12)	119.3(4)
C(28)-H(28)	0.9300	C(8)-C(13)-H(13)	120.4
C(29)-H(29)	0.9300	C(12)-C(13)-H(13)	120.4
C(7)-Au(1)-C(1)	177.38(19)	O(1)-C(14)-C(15)	108.6(4)
C(2)-C(1)-C(6)	113.4(4)	O(1)-C(14)-H(14A)	110.0
C(2)-C(1)-Au(1)	123.4(3)	C(15)-C(14)-H(14A)	110.0
C(6)-C(1)-Au(1)	123.2(4)	O(1)-C(14)-H(14B)	110.0
C(3)-C(2)-F(1)	117.7(5)	C(15)-C(14)-H(14B)	110.0
C(3)-C(2)-C(1)	124.4(4)	H(14A)-C(14)-H(14B)	108.3
F(1)-C(2)-C(1)	117.9(5)	C(14)-C(15)-C(16)	115.4(4)
C(2)-C(3)-F(2)	121.6(5)	C(14)-C(15)-H(15A)	108.4
C(2)-C(3)-C(4)	120.3(5)	C(16)-C(15)-H(15A)	108.4
F(2)-C(3)-C(4)	118.2(5)	C(14)-C(15)-H(15B)	108.4
F(3)-C(4)-C(3)	121.1(5)	C(16)-C(15)-H(15B)	108.4
F(3)-C(4)-C(5)	120.1(5)	H(15A)-C(15)-H(15B)	107.5

C(17)-C(16)-C(15)	115.0(4)	C(24)-C(23)-C(22)	121.7(5)
C(17)-C(16)-H(16A)	108.5	C(24)-C(23)-H(23)	119.2
C(15)-C(16)-H(16A)	108.5	C(22)-C(23)-H(23)	119.2
C(17)-C(16)-H(16B)	108.5	C(25)-C(24)-C(23)	120.6(5)
C(15)-C(16)-H(16B)	108.5	C(25)-C(24)-H(24)	119.7
H(16A)-C(16)-H(16B)	107.5	C(23)-C(24)-H(24)	119.7
N(2)-C(17)-C(16)	111.8(4)	C(24)-C(25)-C(20)	119.7(5)
N(2)-C(17)-H(17A)	109.3	C(24)-C(25)-H(25)	120.2
C(16)-C(17)-H(17A)	109.3	C(20)-C(25)-H(25)	120.2
N(2)-C(17)-H(17B)	109.3	C(27)-C(26)-C(18)	117.1(5)
C(16)-C(17)-H(17B)	109.3	C(27)-C(26)-H(26)	121.4
H(17A)-C(17)-H(17B)	107.9	C(18)-C(26)-H(26)	121.4
N(2)-C(18)-C(26)	129.2(4)	C(26)-C(27)-C(28)	120.9(6)
N(2)-C(18)-C(19)	108.7(4)	C(26)-C(27)-H(27)	119.6
C(26)-C(18)-C(19)	122.1(4)	C(28)-C(27)-H(27)	119.6
C(29)-C(19)-C(18)	118.8(5)	C(29)-C(28)-C(27)	122.0(5)
C(29)-C(19)-C(20)	133.9(5)	C(29)-C(28)-H(28)	119.0
C(18)-C(19)-C(20)	107.2(4)	C(27)-C(28)-H(28)	119.0
C(25)-C(20)-C(21)	119.4(4)	C(28)-C(29)-C(19)	119.1(5)
C(25)-C(20)-C(19)	134.2(5)	C(28)-C(29)-H(29)	120.5
C(21)-C(20)-C(19)	106.4(4)	C(19)-C(29)-H(29)	120.5
N(2)-C(21)-C(22)	129.5(4)	C(7)-N(1)-C(8)	177.7(5)
N(2)-C(21)-C(20)	109.2(4)	C(18)-N(2)-C(21)	108.5(4)
C(22)-C(21)-C(20)	121.3(4)	C(18)-N(2)-C(17)	125.8(4)
C(21)-C(22)-C(23)	117.2(5)	C(21)-N(2)-C(17)	125.0(4)
C(21)-C(22)-H(22)	121.4	C(11)-O(1)-C(14)	117.2(4)
C(23)-C(22)-H(22)	121.4		

Table S8. Bond lengths [\AA] and angles [$^\circ$] of **4**.

Au(1)-C(7)	1.967(12)	C(4)-F(3)	1.355(14)
Au(1)-C(1)	2.004(11)	C(4)-C(5)	1.378(18)
Au(1)-Au(1)#1	3.1262(11)	C(5)-C(6)	1.355(17)
C(1)-C(6)	1.390(16)	C(5)-F(4)	1.358(14)
C(1)-C(2)	1.412(17)	C(6)-F(5)	1.351(13)
C(2)-F(1)	1.373(13)	C(7)-N(3)	1.145(15)
C(2)-C(3)	1.378(18)	C(8)-C(9)	1.346(18)
C(3)-F(2)	1.320(15)	C(8)-C(13)	1.366(17)
C(3)-C(4)	1.357(19)	C(8)-N(3)	1.413(15)

C(9)-C(10)	1.390(17)	C(25)-C(30)	1.414(15)
C(9)-H(9)	0.9300	C(26)-C(27)	1.352(19)
C(10)-C(11)	1.375(17)	C(26)-H(26)	0.9300
C(10)-H(10)	0.9300	C(27)-C(28)	1.39(2)
C(11)-O(1)	1.357(14)	C(27)-H(27)	0.9300
C(11)-C(12)	1.386(17)	C(28)-C(29)	1.367(19)
C(12)-C(13)	1.396(17)	C(28)-H(28)	0.9300
C(12)-H(12)	0.9300	C(29)-C(30)	1.355(18)
C(13)-H(13)	0.9300	C(29)-H(29)	0.9300
C(14)-O(1)	1.458(15)	C(30)-N(1)	1.413(15)
C(14)-C(15)	1.500(17)	C(7)-Au(1)-C(1)	175.4(5)
C(14)-H(14A)	0.9700	C(7)-Au(1)-Au(1)#1	76.7(4)
C(14)-H(14B)	0.9700	C(1)-Au(1)-Au(1)#1	99.5(3)
C(15)-C(16)	1.531(17)	C(6)-C(1)-C(2)	111.7(10)
C(15)-H(15A)	0.9700	C(6)-C(1)-Au(1)	125.3(10)
C(15)-H(15B)	0.9700	C(2)-C(1)-Au(1)	122.8(8)
C(16)-C(17)	1.534(18)	F(1)-C(2)-C(3)	116.8(11)
C(16)-H(16A)	0.9700	F(1)-C(2)-C(1)	118.1(10)
C(16)-H(16B)	0.9700	C(3)-C(2)-C(1)	125.1(11)
C(17)-C(18)	1.491(18)	F(2)-C(3)-C(4)	120.9(12)
C(17)-H(17A)	0.9700	F(2)-C(3)-C(2)	121.4(12)
C(17)-H(17B)	0.9700	C(4)-C(3)-C(2)	117.8(12)
C(18)-N(1)	1.469(14)	F(3)-C(4)-C(3)	119.9(12)
C(18)-H(18A)	0.9700	F(3)-C(4)-C(5)	118.7(12)
C(18)-H(18B)	0.9700	C(3)-C(4)-C(5)	121.4(11)
C(19)-N(1)	1.369(15)	C(6)-C(5)-F(4)	120.9(12)
C(19)-C(20)	1.389(17)	C(6)-C(5)-C(4)	118.1(11)
C(19)-C(24)	1.400(16)	F(4)-C(5)-C(4)	120.9(11)
C(20)-C(21)	1.38(2)	F(5)-C(6)-C(5)	117.0(11)
C(20)-H(20)	0.9300	F(5)-C(6)-C(1)	117.0(11)
C(21)-C(22)	1.42(2)	C(5)-C(6)-C(1)	125.9(12)
C(21)-H(21)	0.9300	N(3)-C(7)-Au(1)	174.0(12)
C(22)-C(23)	1.355(18)	C(9)-C(8)-C(13)	121.6(11)
C(22)-H(22)	0.9300	C(9)-C(8)-N(3)	121.6(12)
C(23)-C(24)	1.404(17)	C(13)-C(8)-N(3)	116.7(11)
C(23)-H(23)	0.9300	C(8)-C(9)-C(10)	121.0(12)
C(24)-C(25)	1.428(16)	C(8)-C(9)-H(9)	119.5
C(25)-C(26)	1.406(16)	C(10)-C(9)-H(9)	119.5

C(11)-C(10)-C(9)	118.2(11)	C(17)-C(18)-H(18A)	109.1
C(11)-C(10)-H(10)	120.9	N(1)-C(18)-H(18B)	109.1
C(9)-C(10)-H(10)	120.9	C(17)-C(18)-H(18B)	109.1
O(1)-C(11)-C(10)	125.0(11)	H(18A)-C(18)-H(18B)	107.8
O(1)-C(11)-C(12)	114.1(10)	N(1)-C(19)-C(20)	129.7(11)
C(10)-C(11)-C(12)	120.8(11)	N(1)-C(19)-C(24)	108.1(10)
C(11)-C(12)-C(13)	119.6(11)	C(20)-C(19)-C(24)	122.1(11)
C(11)-C(12)-H(12)	120.2	C(21)-C(20)-C(19)	117.1(13)
C(13)-C(12)-H(12)	120.2	C(21)-C(20)-H(20)	121.5
C(8)-C(13)-C(12)	118.6(11)	C(19)-C(20)-H(20)	121.5
C(8)-C(13)-H(13)	120.7	C(20)-C(21)-C(22)	122.0(13)
C(12)-C(13)-H(13)	120.7	C(20)-C(21)-H(21)	119.0
O(1)-C(14)-C(15)	105.0(10)	C(22)-C(21)-H(21)	119.0
O(1)-C(14)-H(14A)	110.7	C(23)-C(22)-C(21)	119.1(14)
C(15)-C(14)-H(14A)	110.7	C(23)-C(22)-H(22)	120.4
O(1)-C(14)-H(14B)	110.7	C(21)-C(22)-H(22)	120.4
C(15)-C(14)-H(14B)	110.7	C(22)-C(23)-C(24)	120.7(13)
H(14A)-C(14)-H(14B)	108.8	C(22)-C(23)-H(23)	119.6
C(14)-C(15)-C(16)	110.6(11)	C(24)-C(23)-H(23)	119.6
C(14)-C(15)-H(15A)	109.5	C(19)-C(24)-C(23)	118.6(11)
C(16)-C(15)-H(15A)	109.5	C(19)-C(24)-C(25)	108.0(10)
C(14)-C(15)-H(15B)	109.5	C(23)-C(24)-C(25)	133.3(11)
C(16)-C(15)-H(15B)	109.5	C(26)-C(25)-C(30)	117.5(11)
H(15A)-C(15)-H(15B)	108.1	C(26)-C(25)-C(24)	135.3(11)
C(15)-C(16)-C(17)	112.8(11)	C(30)-C(25)-C(24)	107.2(10)
C(15)-C(16)-H(16A)	109.0	C(27)-C(26)-C(25)	120.0(12)
C(17)-C(16)-H(16A)	109.0	C(27)-C(26)-H(26)	120.0
C(15)-C(16)-H(16B)	109.0	C(25)-C(26)-H(26)	120.0
C(17)-C(16)-H(16B)	109.0	C(26)-C(27)-C(28)	120.1(12)
H(16A)-C(16)-H(16B)	107.8	C(26)-C(27)-H(27)	119.9
C(18)-C(17)-C(16)	113.3(11)	C(28)-C(27)-H(27)	119.9
C(18)-C(17)-H(17A)	108.9	C(29)-C(28)-C(27)	122.1(14)
C(16)-C(17)-H(17A)	108.9	C(29)-C(28)-H(28)	119.0
C(18)-C(17)-H(17B)	108.9	C(27)-C(28)-H(28)	119.0
C(16)-C(17)-H(17B)	108.9	C(30)-C(29)-C(28)	117.7(13)
H(17A)-C(17)-H(17B)	107.7	C(30)-C(29)-H(29)	121.2
N(1)-C(18)-C(17)	112.6(10)	C(28)-C(29)-H(29)	121.2
N(1)-C(18)-H(18A)	109.1	C(29)-C(30)-N(1)	130.7(11)

C(29)-C(30)-C(25)	122.6(11)	C(30)-N(1)-C(18)	123.2(10)
N(1)-C(30)-C(25)	106.7(10)	C(7)-N(3)-C(8)	176.4(14)
C(19)-N(1)-C(30)	110.0(9)	C(11)-O(1)-C(14)	118.1(9)
C(19)-N(1)-C(18)	126.8(10)		

Table S9. Bond lengths [\AA] and angles [$^\circ$] of **5**.

Au(1)-C(25)	1.962(7)	C(12)-N(2)	1.463(6)
Au(1)-C(26)	2.017(6)	C(12)-H(12A)	0.9700
C(1)-C(2)	1.365(10)	C(12)-H(12B)	0.9700
C(1)-C(6)	1.397(9)	C(13)-C(14)	1.369(8)
C(1)-N(1)	1.408(8)	C(13)-N(2)	1.387(7)
C(2)-C(3)	1.364(9)	C(13)-C(18)	1.424(7)
C(2)-H(2)	0.9300	C(14)-C(15)	1.374(9)
C(3)-C(4)	1.403(8)	C(14)-H(14)	0.9300
C(3)-H(3)	0.9300	C(15)-C(16)	1.401(10)
C(4)-O(1)	1.361(7)	C(15)-H(15)	0.9300
C(4)-C(5)	1.371(9)	C(16)-C(17)	1.358(9)
C(5)-C(6)	1.389(8)	C(16)-H(16)	0.9300
C(5)-H(5)	0.9300	C(17)-C(18)	1.400(8)
C(6)-H(6)	0.9300	C(17)-H(17)	0.9300
C(7)-O(1)	1.427(7)	C(18)-C(19)	1.445(8)
C(7)-C(8)	1.498(8)	C(19)-C(20)	1.390(8)
C(7)-H(7A)	0.9700	C(19)-C(24)	1.402(7)
C(7)-H(7B)	0.9700	C(20)-C(21)	1.372(9)
C(8)-C(9)	1.507(8)	C(20)-H(20)	0.9300
C(8)-H(8A)	0.9700	C(21)-C(22)	1.371(10)
C(8)-H(8B)	0.9700	C(21)-H(21)	0.9300
C(9)-C(10)	1.506(7)	C(22)-C(23)	1.361(9)
C(9)-H(9A)	0.9700	C(22)-H(22)	0.9300
C(9)-H(9B)	0.9700	C(23)-C(24)	1.380(8)
C(10)-C(11)	1.528(6)	C(23)-H(23)	0.9300
C(10)-H(10A)	0.9700	C(24)-N(2)	1.395(6)
C(10)-H(10B)	0.9700	C(25)-N(1)	1.151(9)
C(11)-C(12)	1.509(7)	C(26)-C(31)	1.372(9)
C(11)-H(11A)	0.9700	C(26)-C(27)	1.395(9)
C(11)-H(11B)	0.9700	C(27)-F(1)	1.333(8)

C(27)-C(28)	1.355(9)	H(8A)-C(8)-H(8B)	107.8
C(28)-C(29)	1.321(12)	C(10)-C(9)-C(8)	114.4(5)
C(28)-F(2)	1.387(8)	C(10)-C(9)-H(9A)	108.7
C(29)-F(3)	1.367(7)	C(8)-C(9)-H(9A)	108.7
C(29)-C(30)	1.374(11)	C(10)-C(9)-H(9B)	108.7
C(30)-F(4)	1.353(8)	C(8)-C(9)-H(9B)	108.7
C(30)-C(31)	1.356(9)	H(9A)-C(9)-H(9B)	107.6
C(31)-F(5)	1.354(7)	C(9)-C(10)-C(11)	113.7(4)
C(25)-Au(1)-C(26)	178.7(2)	C(9)-C(10)-H(10A)	108.8
C(2)-C(1)-C(6)	121.5(6)	C(11)-C(10)-H(10A)	108.8
C(2)-C(1)-N(1)	120.2(6)	C(9)-C(10)-H(10B)	108.8
C(6)-C(1)-N(1)	118.2(6)	C(11)-C(10)-H(10B)	108.8
C(3)-C(2)-C(1)	119.2(6)	H(10A)-C(10)-H(10B)	107.7
C(3)-C(2)-H(2)	120.4	C(12)-C(11)-C(10)	111.5(4)
C(1)-C(2)-H(2)	120.4	C(12)-C(11)-H(11A)	109.3
C(2)-C(3)-C(4)	120.5(6)	C(10)-C(11)-H(11A)	109.3
C(2)-C(3)-H(3)	119.7	C(12)-C(11)-H(11B)	109.3
C(4)-C(3)-H(3)	119.7	C(10)-C(11)-H(11B)	109.3
O(1)-C(4)-C(5)	124.8(5)	H(11A)-C(11)-H(11B)	108.0
O(1)-C(4)-C(3)	114.9(5)	N(2)-C(12)-C(11)	114.4(4)
C(5)-C(4)-C(3)	120.3(6)	N(2)-C(12)-H(12A)	108.7
C(4)-C(5)-C(6)	119.3(6)	C(11)-C(12)-H(12A)	108.7
C(4)-C(5)-H(5)	120.3	N(2)-C(12)-H(12B)	108.7
C(6)-C(5)-H(5)	120.3	C(11)-C(12)-H(12B)	108.7
C(5)-C(6)-C(1)	119.1(6)	H(12A)-C(12)-H(12B)	107.6
C(5)-C(6)-H(6)	120.4	C(14)-C(13)-N(2)	129.5(5)
C(1)-C(6)-H(6)	120.4	C(14)-C(13)-C(18)	122.8(5)
O(1)-C(7)-C(8)	109.1(5)	N(2)-C(13)-C(18)	107.6(4)
O(1)-C(7)-H(7A)	109.9	C(13)-C(14)-C(15)	117.5(5)
C(8)-C(7)-H(7A)	109.9	C(13)-C(14)-H(14)	121.3
O(1)-C(7)-H(7B)	109.9	C(15)-C(14)-H(14)	121.3
C(8)-C(7)-H(7B)	109.9	C(14)-C(15)-C(16)	121.0(6)
H(7A)-C(7)-H(7B)	108.3	C(14)-C(15)-H(15)	119.5
C(7)-C(8)-C(9)	113.1(5)	C(16)-C(15)-H(15)	119.5
C(7)-C(8)-H(8A)	109.0	C(17)-C(16)-C(15)	121.7(6)
C(9)-C(8)-H(8A)	109.0	C(17)-C(16)-H(16)	119.1
C(7)-C(8)-H(8B)	109.0	C(15)-C(16)-H(16)	119.1
C(9)-C(8)-H(8B)	109.0	C(16)-C(17)-C(18)	119.1(5)

C(16)-C(17)-H(17)	120.5	C(31)-C(26)-C(27)	112.9(6)
C(18)-C(17)-H(17)	120.5	C(31)-C(26)-Au(1)	122.9(5)
C(17)-C(18)-C(13)	117.8(5)	C(27)-C(26)-Au(1)	124.2(5)
C(17)-C(18)-C(19)	134.7(5)	F(1)-C(27)-C(28)	117.3(6)
C(13)-C(18)-C(19)	107.4(4)	F(1)-C(27)-C(26)	120.1(6)
C(20)-C(19)-C(24)	118.2(5)	C(28)-C(27)-C(26)	122.7(6)
C(20)-C(19)-C(18)	135.2(5)	C(29)-C(28)-C(27)	121.7(6)
C(24)-C(19)-C(18)	106.6(4)	C(29)-C(28)-F(2)	118.5(6)
C(21)-C(20)-C(19)	119.5(6)	C(27)-C(28)-F(2)	119.7(7)
C(21)-C(20)-H(20)	120.3	C(28)-C(29)-F(3)	121.5(7)
C(19)-C(20)-H(20)	120.3	C(28)-C(29)-C(30)	119.1(6)
C(22)-C(21)-C(20)	120.2(6)	F(3)-C(29)-C(30)	119.4(7)
C(22)-C(21)-H(21)	119.9	F(4)-C(30)-C(31)	120.5(7)
C(20)-C(21)-H(21)	119.9	F(4)-C(30)-C(29)	121.0(6)
C(23)-C(22)-C(21)	122.7(6)	C(31)-C(30)-C(29)	118.5(6)
C(23)-C(22)-H(22)	118.6	F(5)-C(31)-C(30)	116.5(6)
C(21)-C(22)-H(22)	118.6	F(5)-C(31)-C(26)	118.4(6)
C(22)-C(23)-C(24)	117.0(5)	C(30)-C(31)-C(26)	125.1(6)
C(22)-C(23)-H(23)	121.5	C(25)-N(1)-C(1)	179.4(8)
C(24)-C(23)-H(23)	121.5	C(13)-N(2)-C(24)	109.4(4)
C(23)-C(24)-N(2)	128.7(5)	C(13)-N(2)-C(12)	124.7(4)
C(23)-C(24)-C(19)	122.3(5)	C(24)-N(2)-C(12)	125.8(4)
N(2)-C(24)-C(19)	109.0(4)	C(4)-O(1)-C(7)	117.8(5)
N(1)-C(25)-Au(1)	179.1(6)		

Table S10. Bond lengths [\AA] and angles [$^{\circ}$] of **7**.

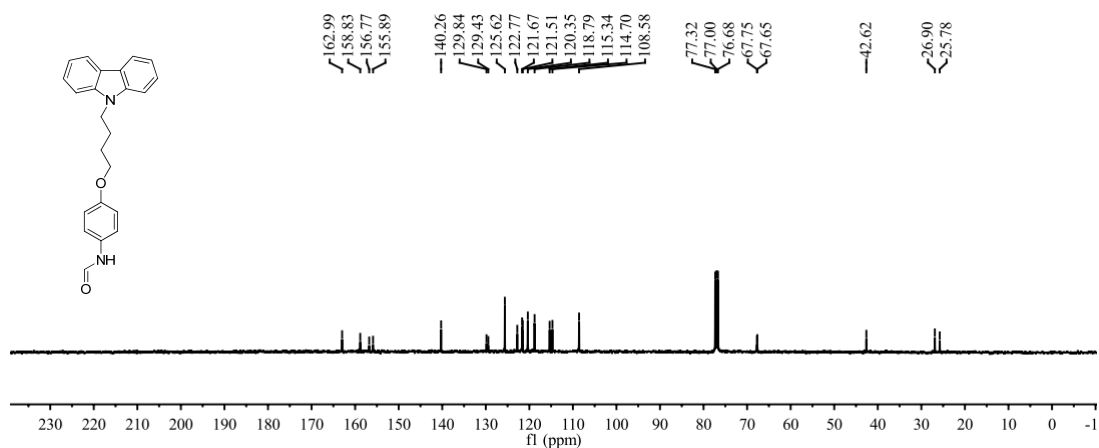
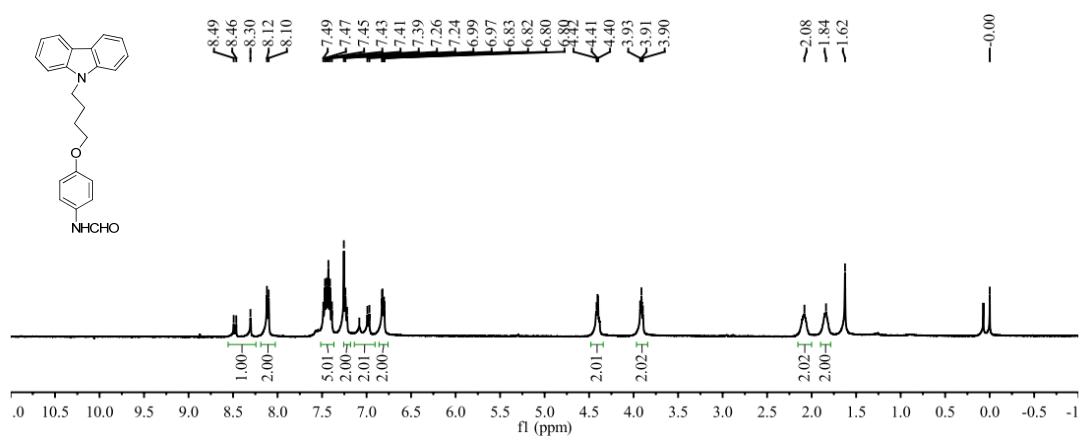
Au(1)-C(7)	1.984(15)	N(2)-C(21)	1.437(15)
Au(1)-C(1)	2.048(12)	C(24)-C(29)	1.402(16)
Au(1)-Au(1)#1	3.3575(14)	C(24)-C(25)	1.413(15)
O(1)-C(11)	1.348(14)	C(24)-C(23)	1.445(16)
O(1)-C(14)	1.428(13)	N(1)-C(7)	1.132(17)
C(15)-C(14)	1.515(16)	N(1)-C(8)	1.415(15)
C(15)-C(16)	1.519(17)	C(12)-C(13)	1.369(18)
C(15)-H(15A)	0.9700	C(12)-C(11)	1.382(18)
C(15)-H(15B)	0.9700	C(12)-H(12)	0.9300
N(2)-C(29)	1.371(14)	C(29)-C(28)	1.393(17)
N(2)-C(22)	1.392(18)	C(11)-C(10)	1.397(18)

C(13)-C(8)	1.356(19)	C(30)-C(31)	1.38(3)
C(13)-H(13)	0.9300	C(30)-H(30)	0.9300
C(21)-C(20)	1.524(17)	C(18)-H(18A)	0.9700
C(21)-H(21A)	0.9700	C(18)-H(18B)	0.9700
C(21)-H(21B)	0.9700	C(2)-F(1)	1.364(18)
C(23)-C(33)	1.391(18)	C(2)-C(3)	1.38(2)
C(23)-C(22)	1.392(17)	C(3)-C(4)	1.33(2)
C(14)-H(14A)	0.9700	C(10)-H(10)	0.9300
C(14)-H(14B)	0.9700	C(4)-C(5)	1.388(19)
F(2)-C(3)	1.343(14)	C(31)-C(32)	1.39(3)
C(22)-C(30)	1.396(17)	C(31)-H(31)	0.9300
C(16)-C(17)	1.510(16)	C(5)-F(4)	1.313(17)
C(16)-H(16A)	0.9700	C(33)-C(32)	1.36(2)
C(16)-H(16B)	0.9700	C(33)-H(33)	0.9300
C(9)-C(10)	1.360(18)	C(32)-H(32)	0.9300
C(9)-C(8)	1.36(2)	C(7)-Au(1)-C(1)	176.0(6)
C(9)-H(9)	0.9300	C(7)-Au(1)-Au(1)#1	93.4(5)
C(26)-C(25)	1.363(18)	C(1)-Au(1)-Au(1)#1	88.4(4)
C(26)-C(27)	1.38(2)	C(11)-O(1)-C(14)	118.0(9)
C(26)-H(26)	0.9300	C(14)-C(15)-C(16)	111.8(10)
C(25)-H(25)	0.9300	C(14)-C(15)-H(15A)	109.2
C(19)-C(20)	1.499(17)	C(16)-C(15)-H(15A)	109.2
C(19)-C(18)	1.533(17)	C(14)-C(15)-H(15B)	109.2
C(19)-H(19A)	0.9700	C(16)-C(15)-H(15B)	109.2
C(19)-H(19B)	0.9700	H(15A)-C(15)-H(15B)	107.9
C(28)-C(27)	1.389(18)	C(29)-N(2)-C(22)	108.1(10)
C(28)-H(28)	0.9300	C(29)-N(2)-C(21)	126.1(11)
F(3)-C(4)	1.358(14)	C(22)-N(2)-C(21)	125.8(11)
C(6)-C(1)	1.34(2)	C(29)-C(24)-C(25)	119.4(11)
C(6)-F(5)	1.356(13)	C(29)-C(24)-C(23)	106.8(9)
C(6)-C(5)	1.39(2)	C(25)-C(24)-C(23)	133.8(11)
C(1)-C(2)	1.347(19)	C(7)-N(1)-C(8)	170.8(16)
C(27)-H(27)	0.9300	C(13)-C(12)-C(11)	120.3(13)
C(17)-C(18)	1.530(17)	C(13)-C(12)-H(12)	119.9
C(17)-H(17A)	0.9700	C(11)-C(12)-H(12)	119.9
C(17)-H(17B)	0.9700	N(2)-C(29)-C(28)	128.7(11)
C(20)-H(20A)	0.9700	N(2)-C(29)-C(24)	109.4(10)
C(20)-H(20B)	0.9700	C(28)-C(29)-C(24)	121.9(10)

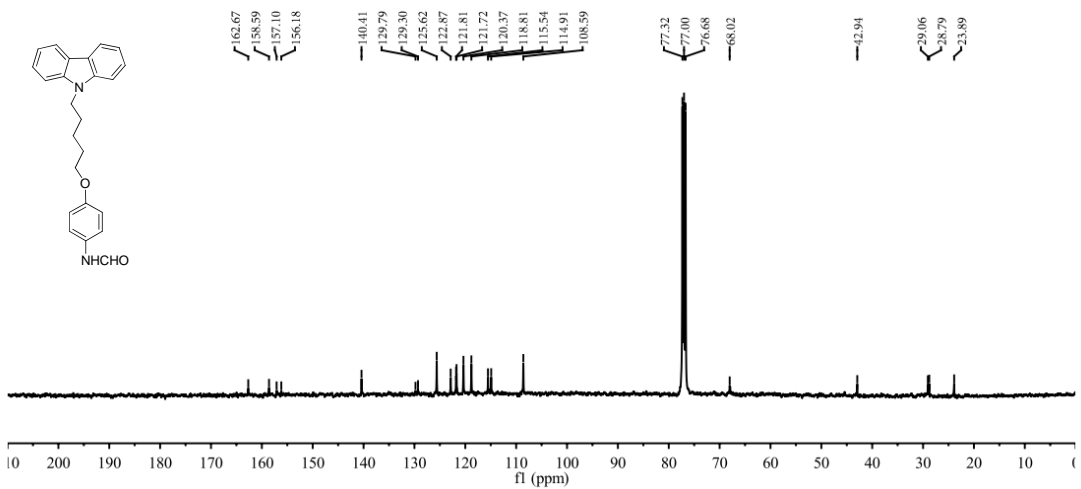
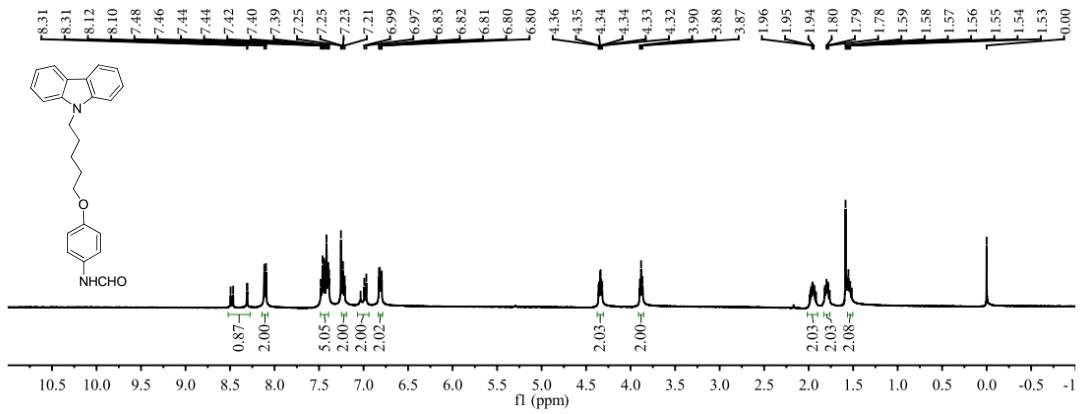
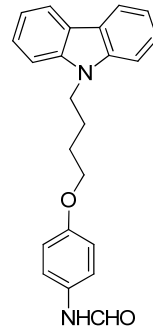
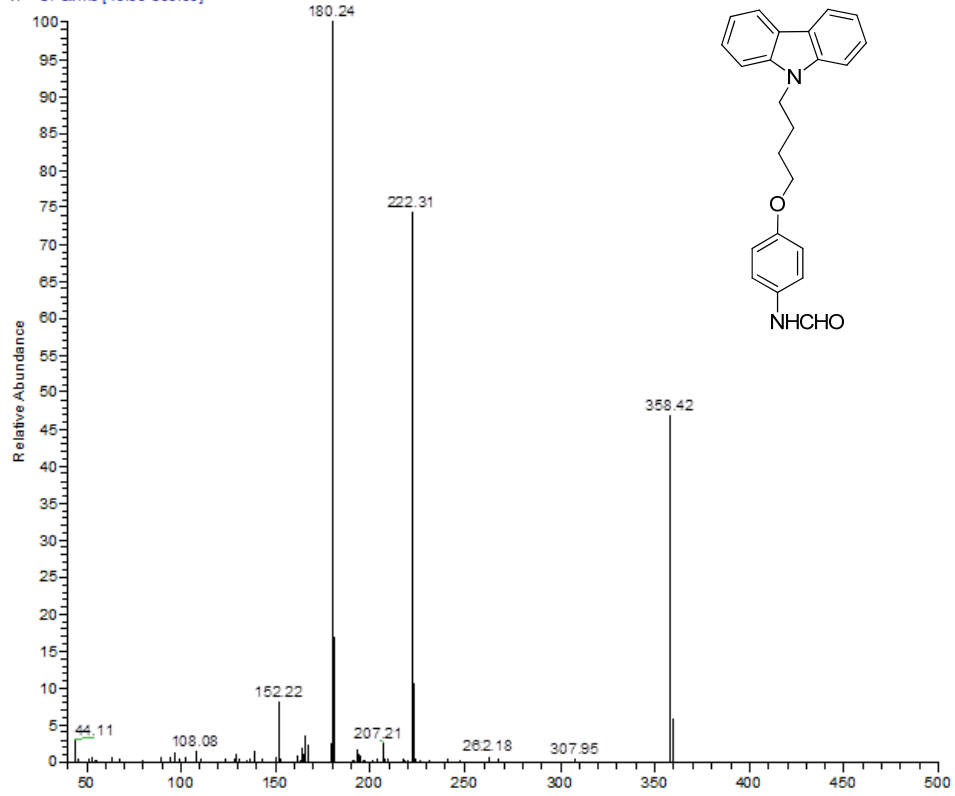
O(1)-C(11)-C(12)	126.0(11)	C(26)-C(25)-H(25)	120.9
O(1)-C(11)-C(10)	114.8(11)	C(24)-C(25)-H(25)	120.9
C(12)-C(11)-C(10)	119.2(11)	C(20)-C(19)-C(18)	111.7(10)
C(8)-C(13)-C(12)	119.7(13)	C(20)-C(19)-H(19A)	109.3
C(8)-C(13)-H(13)	120.1	C(18)-C(19)-H(19A)	109.3
C(12)-C(13)-H(13)	120.1	C(20)-C(19)-H(19B)	109.3
N(1)-C(7)-Au(1)	170.5(15)	C(18)-C(19)-H(19B)	109.3
N(2)-C(21)-C(20)	112.9(10)	H(19A)-C(19)-H(19B)	107.9
N(2)-C(21)-H(21A)	109.0	C(27)-C(28)-C(29)	116.9(12)
C(20)-C(21)-H(21A)	109.0	C(27)-C(28)-H(28)	121.6
N(2)-C(21)-H(21B)	109.0	C(29)-C(28)-H(28)	121.6
C(20)-C(21)-H(21B)	109.0	C(1)-C(6)-F(5)	118.0(12)
H(21A)-C(21)-H(21B)	107.8	C(1)-C(6)-C(5)	126.6(12)
C(33)-C(23)-C(22)	120.0(12)	F(5)-C(6)-C(5)	115.4(14)
C(33)-C(23)-C(24)	133.8(12)	C(6)-C(1)-C(2)	114.8(12)
C(22)-C(23)-C(24)	106.1(10)	C(6)-C(1)-Au(1)	122.0(9)
O(1)-C(14)-C(15)	107.5(10)	C(2)-C(1)-Au(1)	123.2(11)
O(1)-C(14)-H(14A)	110.2	C(26)-C(27)-C(28)	121.7(12)
C(15)-C(14)-H(14A)	110.2	C(26)-C(27)-H(27)	119.2
O(1)-C(14)-H(14B)	110.2	C(28)-C(27)-H(27)	119.2
C(15)-C(14)-H(14B)	110.2	C(16)-C(17)-C(18)	113.1(11)
H(14A)-C(14)-H(14B)	108.5	C(16)-C(17)-H(17A)	109.0
C(23)-C(22)-N(2)	109.6(10)	C(18)-C(17)-H(17A)	109.0
C(23)-C(22)-C(30)	121.2(14)	C(16)-C(17)-H(17B)	109.0
N(2)-C(22)-C(30)	129.1(14)	C(18)-C(17)-H(17B)	109.0
C(17)-C(16)-C(15)	114.1(11)	H(17A)-C(17)-H(17B)	107.8
C(17)-C(16)-H(16A)	108.7	C(19)-C(20)-C(21)	111.5(10)
C(15)-C(16)-H(16A)	108.7	C(19)-C(20)-H(20A)	109.3
C(17)-C(16)-H(16B)	108.7	C(21)-C(20)-H(20A)	109.3
C(15)-C(16)-H(16B)	108.7	C(19)-C(20)-H(20B)	109.3
H(16A)-C(16)-H(16B)	107.6	C(21)-C(20)-H(20B)	109.3
C(10)-C(9)-C(8)	120.6(13)	H(20A)-C(20)-H(20B)	108.0
C(10)-C(9)-H(9)	119.7	C(31)-C(30)-C(22)	117.1(16)
C(8)-C(9)-H(9)	119.7	C(31)-C(30)-H(30)	121.4
C(25)-C(26)-C(27)	121.9(11)	C(22)-C(30)-H(30)	121.4
C(25)-C(26)-H(26)	119.0	C(17)-C(18)-C(19)	115.4(11)
C(27)-C(26)-H(26)	119.0	C(17)-C(18)-H(18A)	108.4
C(26)-C(25)-C(24)	118.2(12)	C(19)-C(18)-H(18A)	108.4

C(17)-C(18)-H(18B)	108.4	C(3)-C(4)-F(3)	121.0(13)
C(19)-C(18)-H(18B)	108.4	C(3)-C(4)-C(5)	121.7(13)
H(18A)-C(18)-H(18B)	107.5	F(3)-C(4)-C(5)	117.2(15)
C(1)-C(2)-F(1)	120.5(13)	C(30)-C(31)-C(32)	121.8(13)
C(1)-C(2)-C(3)	123.2(14)	C(30)-C(31)-H(31)	119.1
F(1)-C(2)-C(3)	116.1(13)	C(32)-C(31)-H(31)	119.1
C(4)-C(3)-F(2)	119.1(13)	F(4)-C(5)-C(6)	123.1(13)
C(4)-C(3)-C(2)	119.2(12)	F(4)-C(5)-C(4)	122.4(14)
F(2)-C(3)-C(2)	121.6(15)	C(6)-C(5)-C(4)	114.4(14)
C(9)-C(10)-C(11)	119.2(13)	C(32)-C(33)-C(23)	118.9(15)
C(9)-C(10)-H(10)	120.4	C(32)-C(33)-H(33)	120.6
C(11)-C(10)-H(10)	120.4	C(23)-C(33)-H(33)	120.6
C(13)-C(8)-C(9)	120.9(11)	C(33)-C(32)-C(31)	120.9(15)
C(13)-C(8)-N(1)	121.6(13)	C(33)-C(32)-H(32)	119.6
C(9)-C(8)-N(1)	117.4(12)	C(31)-C(32)-H(32)	119.6

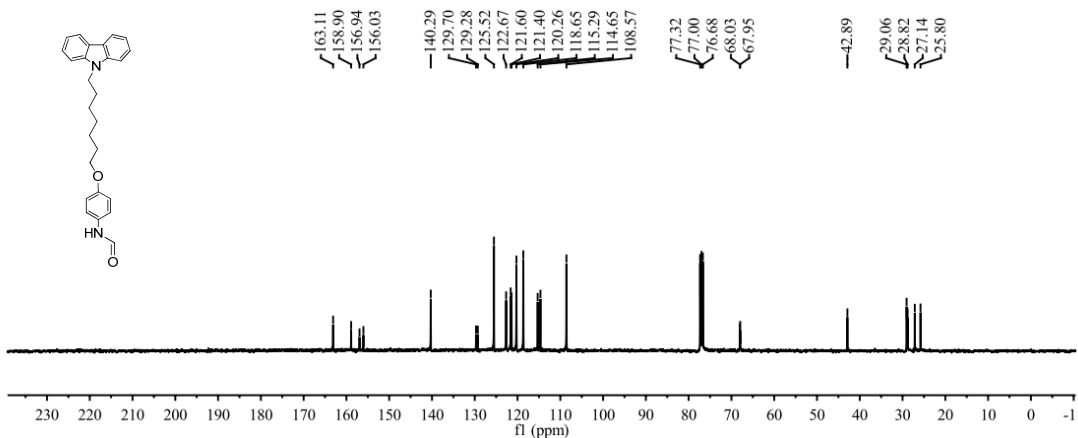
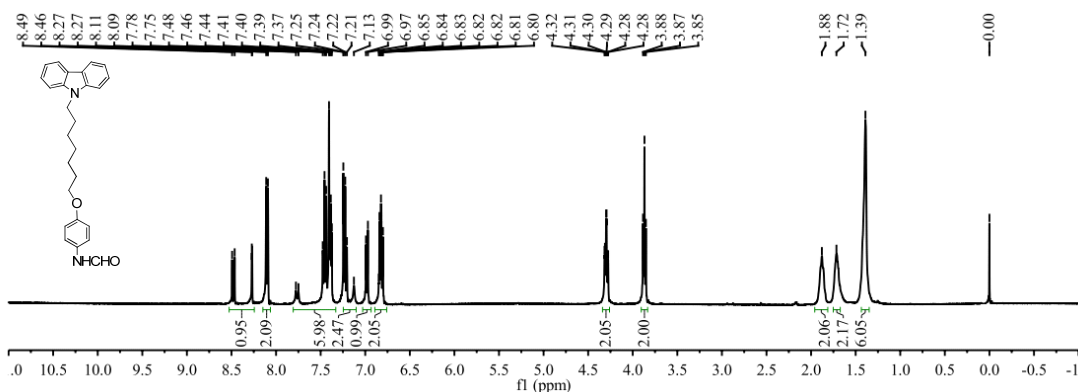
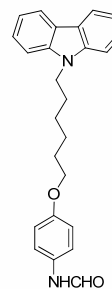
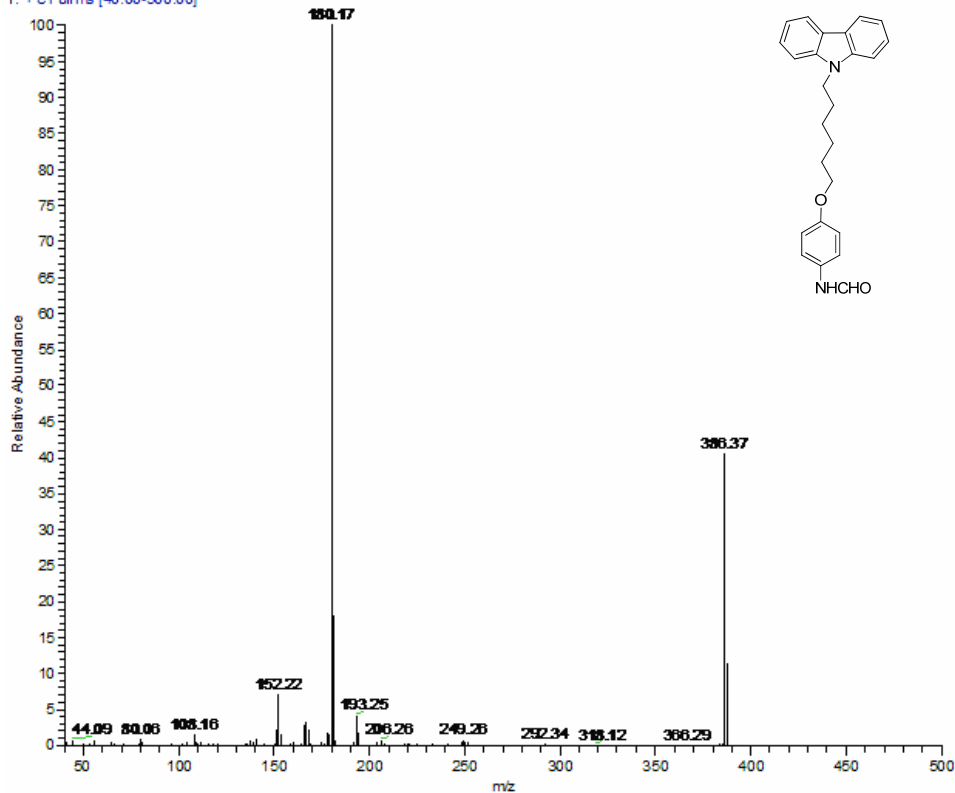
Copies of NMR spectra and Mass spectra



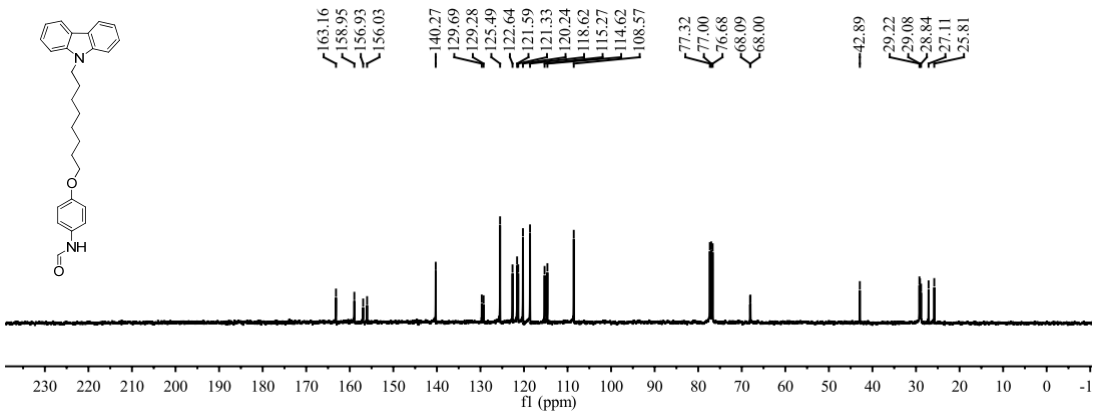
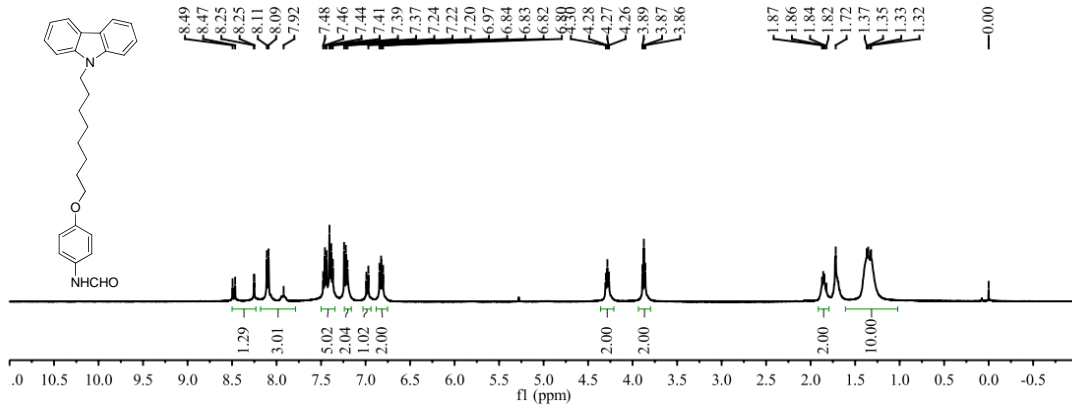
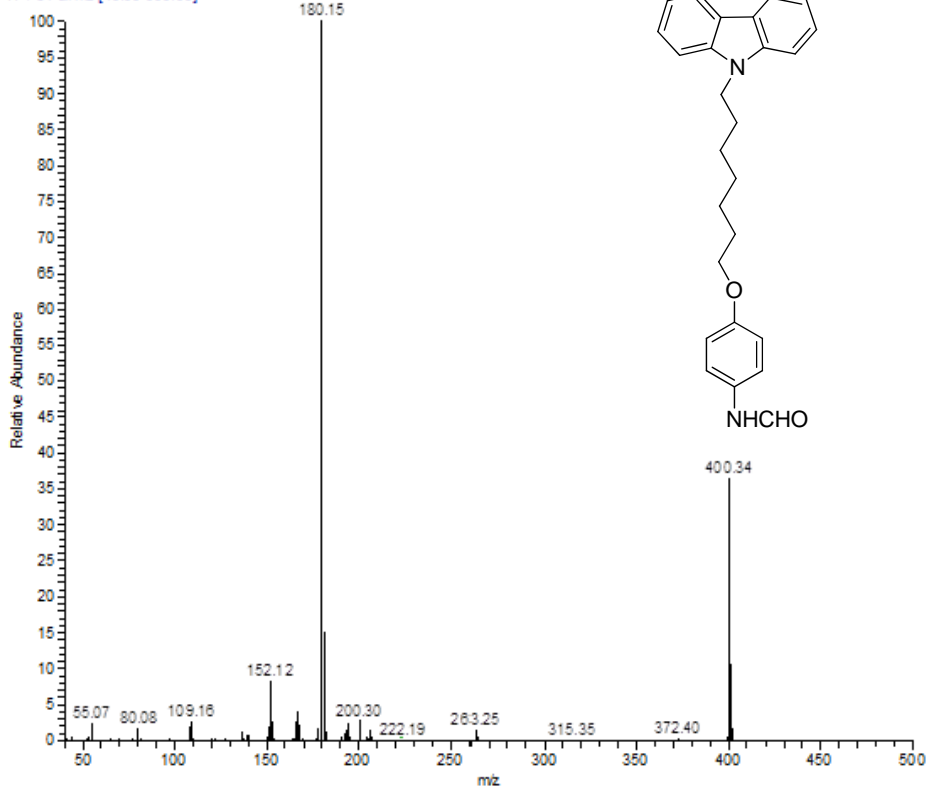
CZ308 #650 RT: 3.03 AV: 1 SB: 732 0.14-2.88, 3.31-3.93 NL: 0.45E4
 T: + cFull.ms [40.00-500.00]



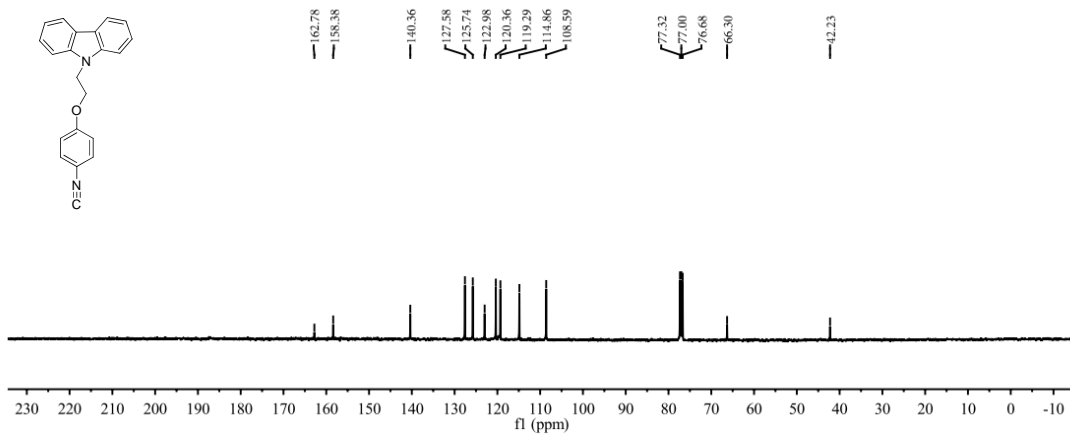
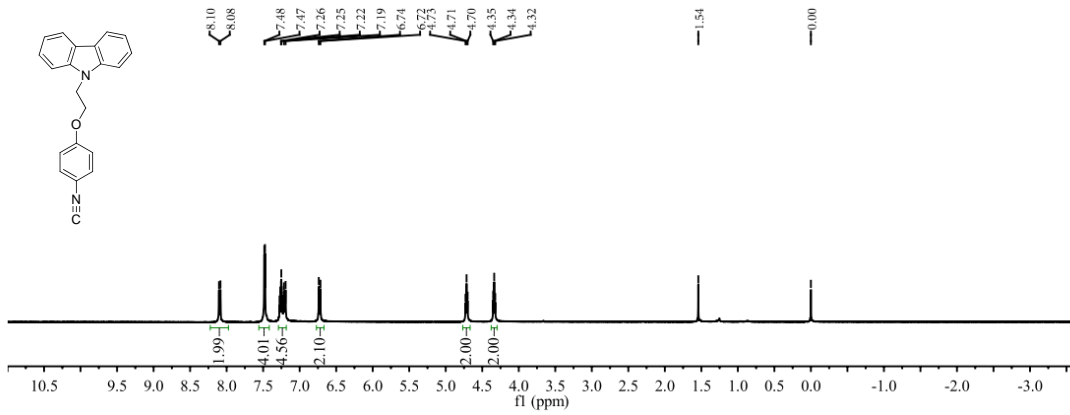
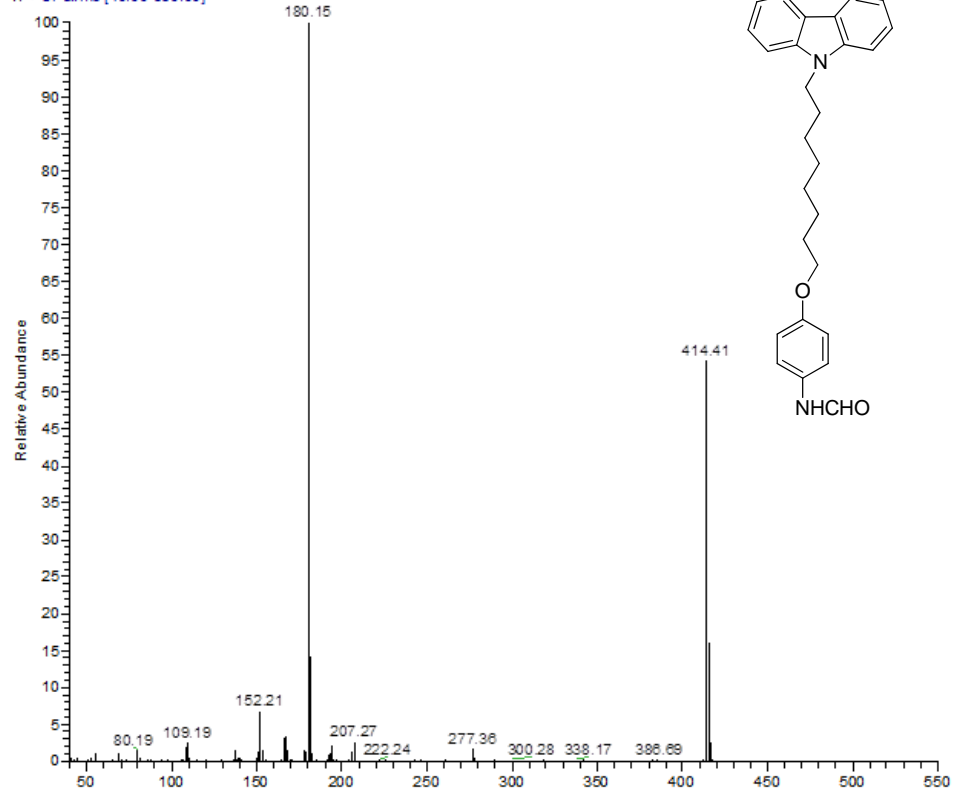
CZ235 #677 RT: 3.15 AV: 1 SB: 749 0.04-2.92, 3.44-4.00 NL: 3.45E5
 T: +c Full ms [40.00-500.00]



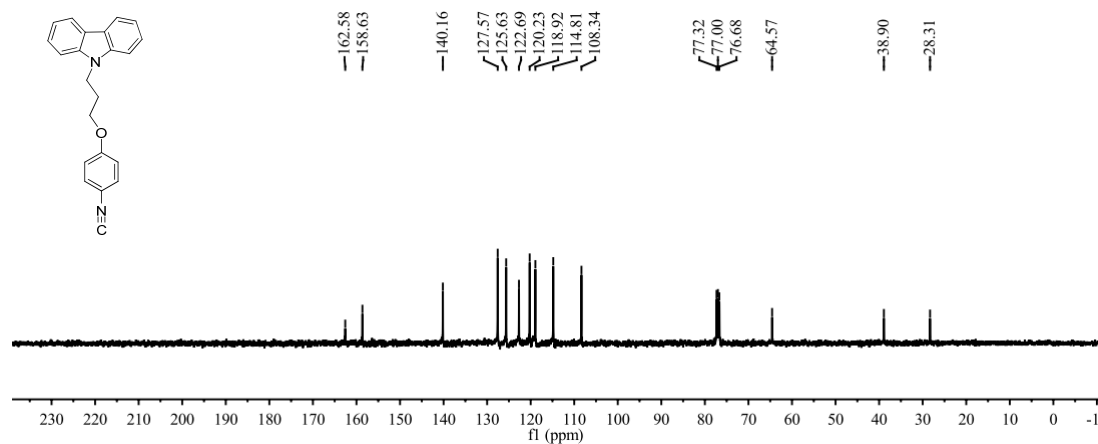
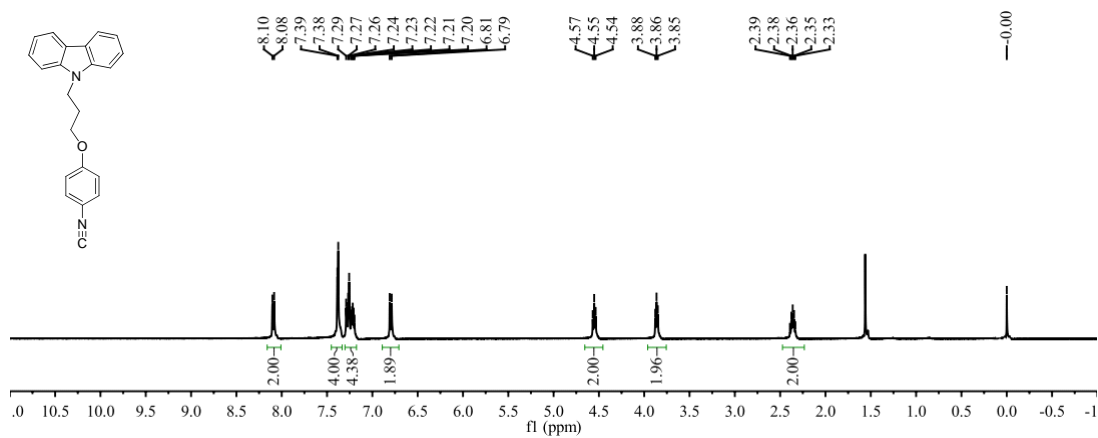
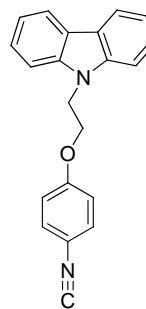
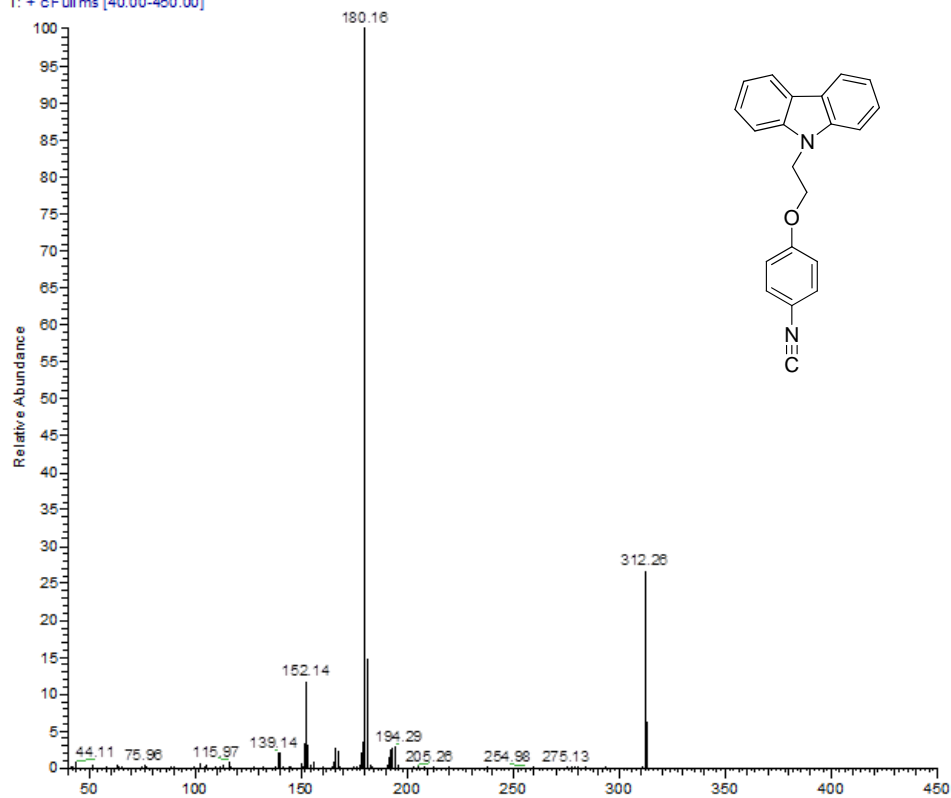
CZ373 #560 RT: 3.43 AV: 1 SB: 422 1.34-3.04, 3.80-4.33 NL: 4.07E6
 T: +c Fullms [40.00-500.00]



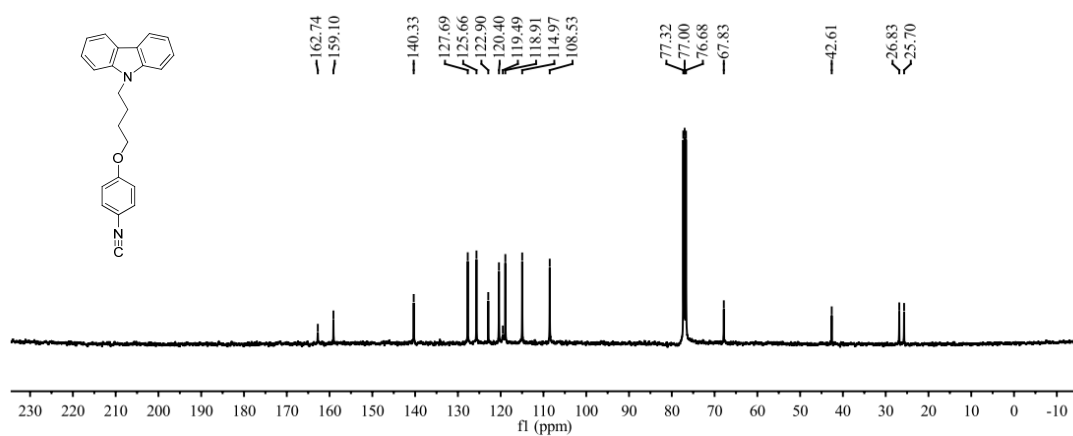
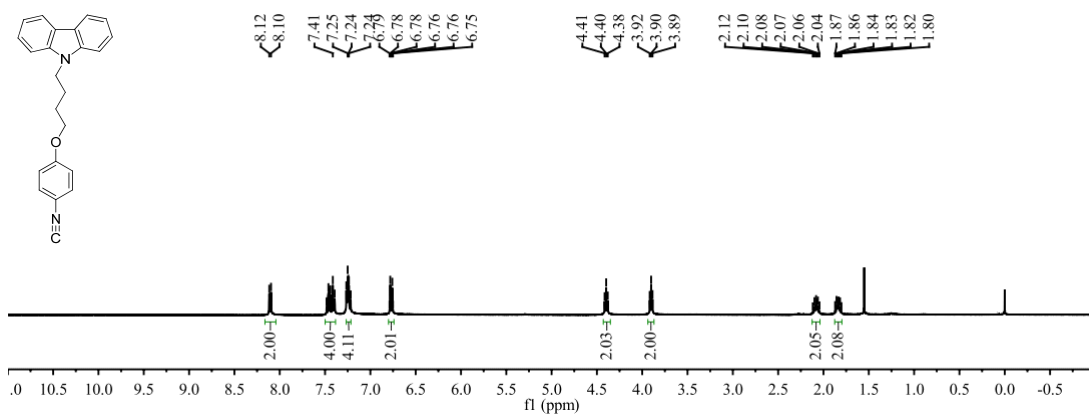
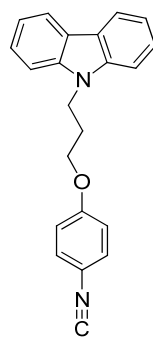
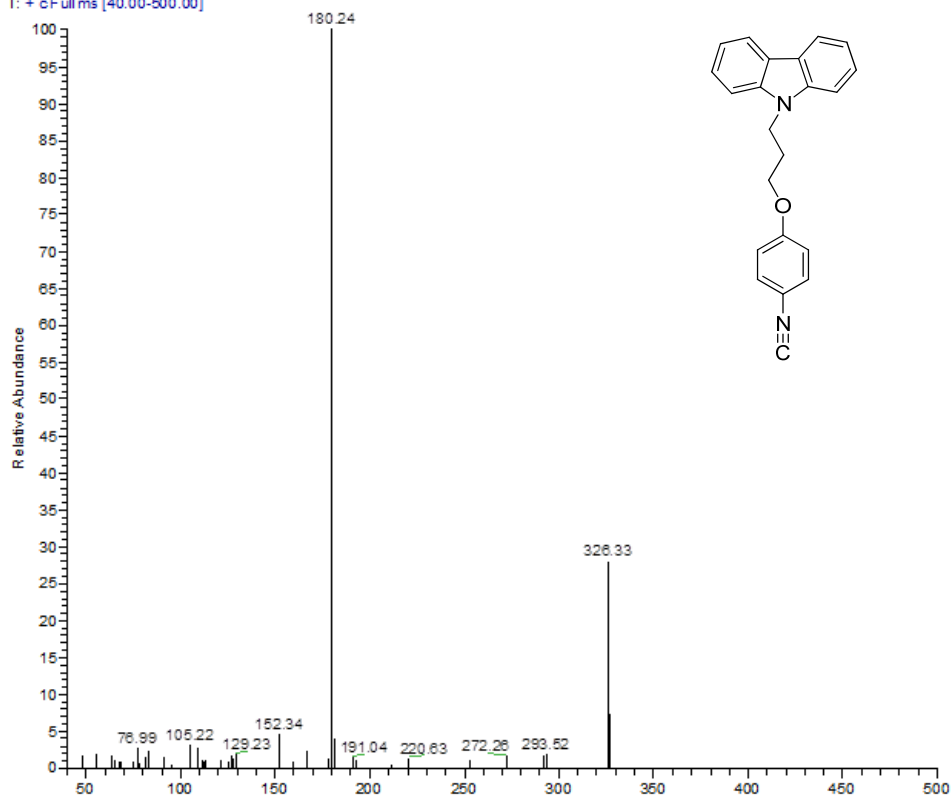
CZ309 #547 RT: 2.81 AV: 1 SB: 589 0.07-2.52, 3.00-3.53 NL: 1.20E6
 T: + cFull.ms [40.00-550.00]



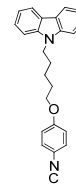
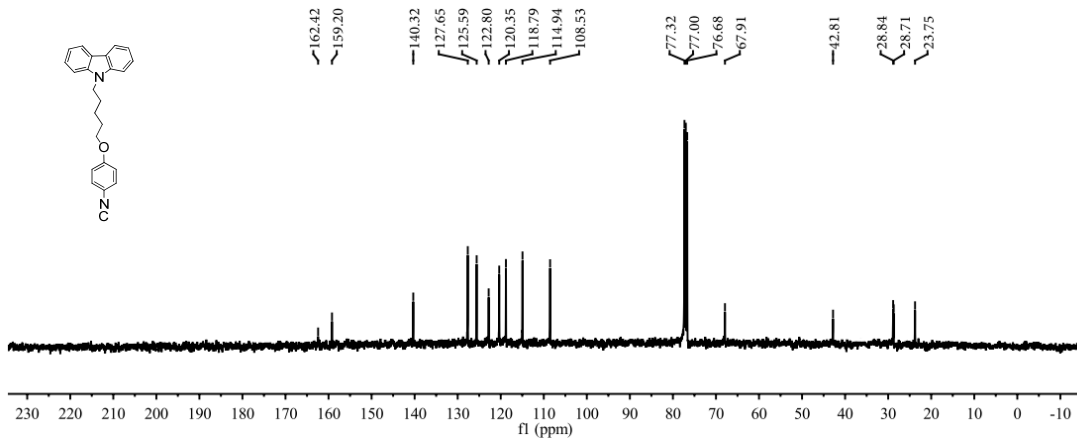
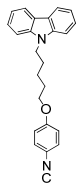
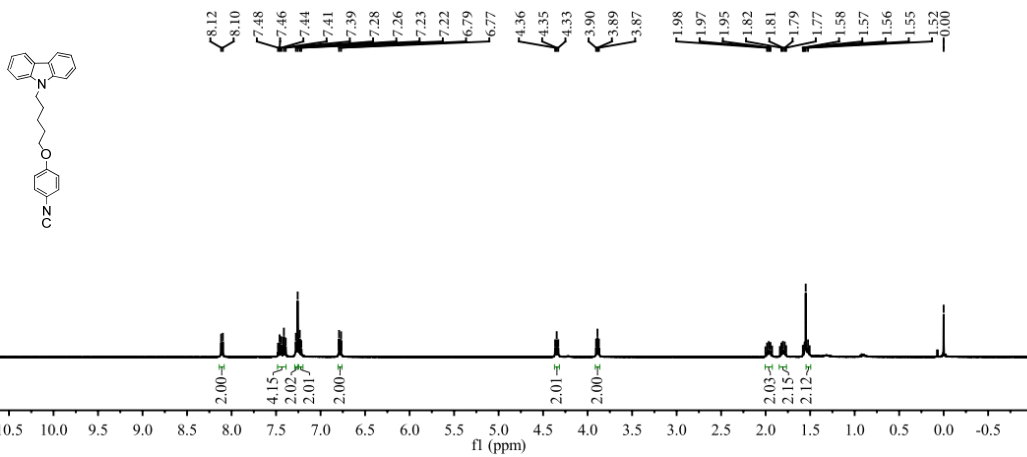
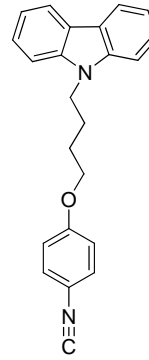
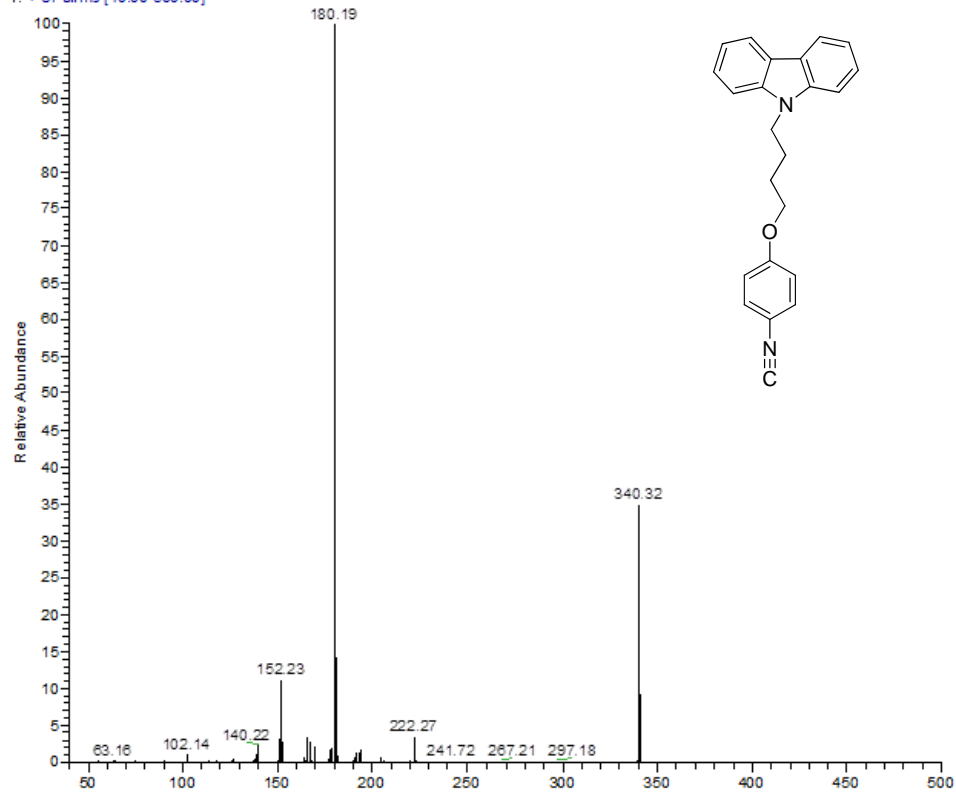
CZ325 #504 RT: 2.12 AV: 1 SB: 532 0.04-1.94, 2.37-2.67 NL: 4.75E5
 T: + cFull.ms [40.00-450.00]



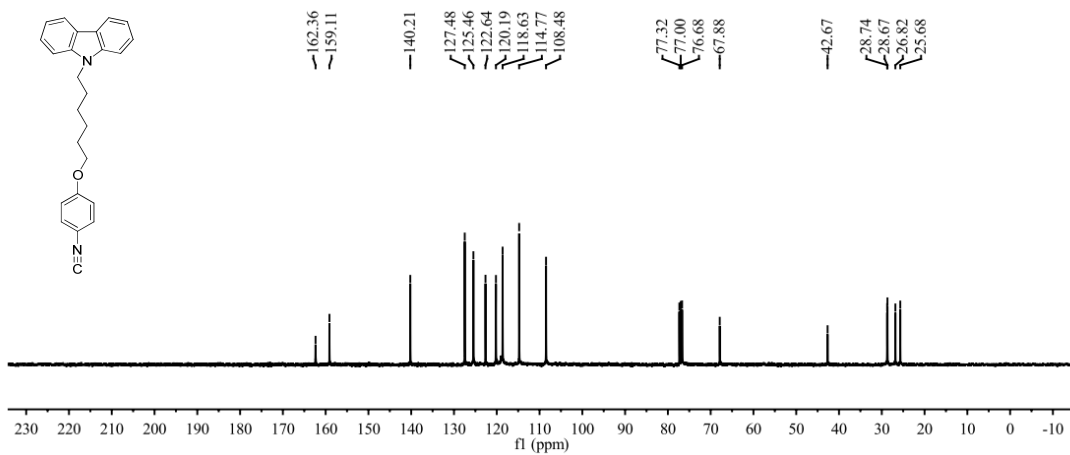
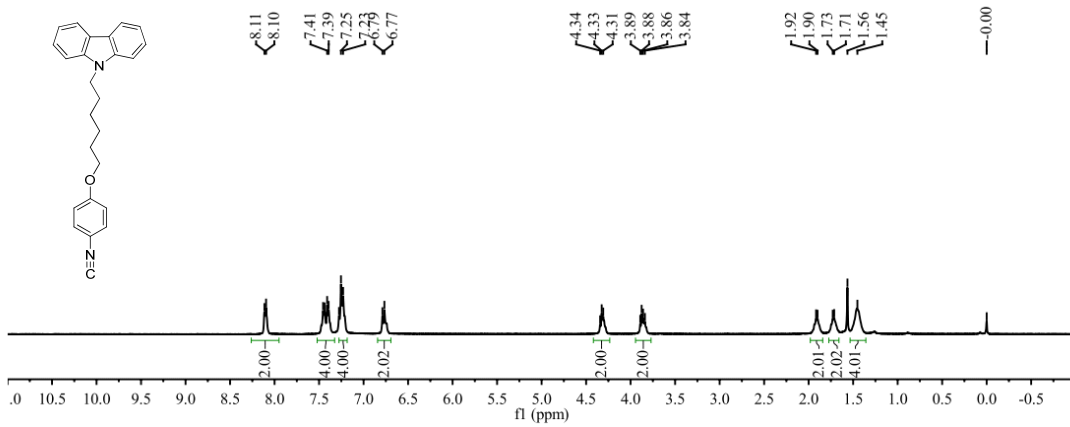
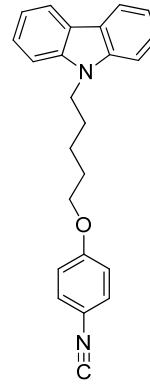
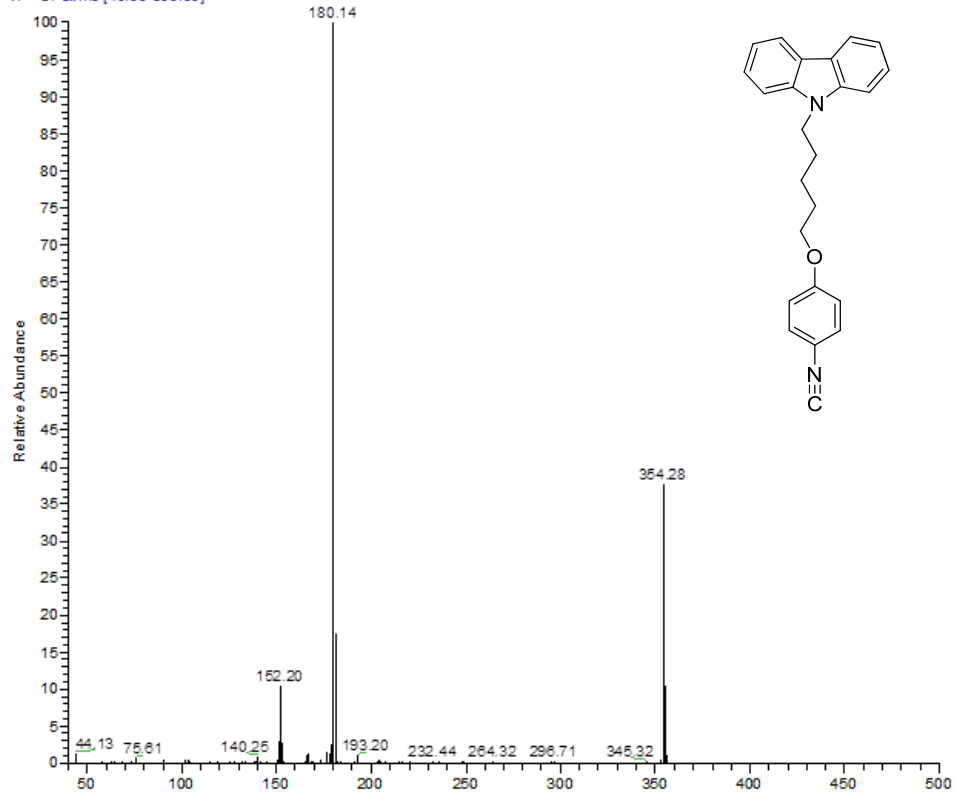
CZ369 #275 RT: 2.06 AV: 1 SB: 228 0.47-1.79 , 2.55-3.02 NL: 2.01E4
 T: + cFullms [40.00-500.00]



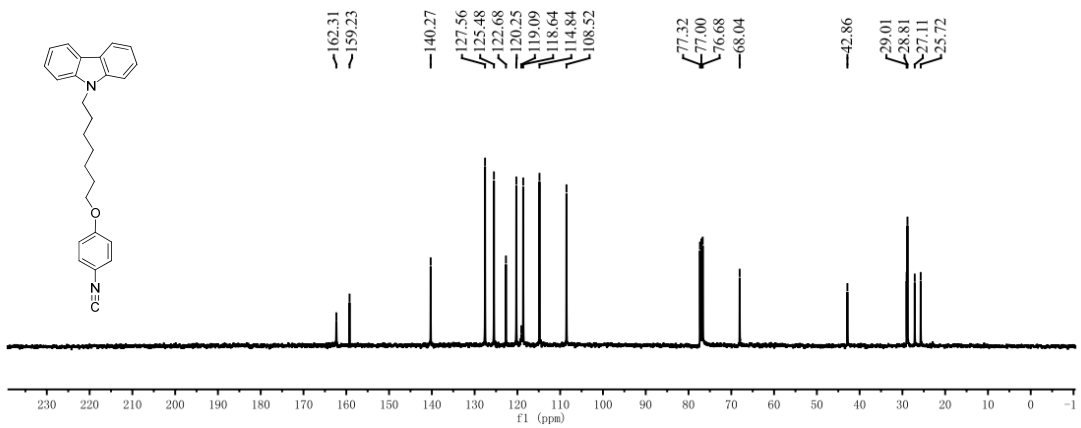
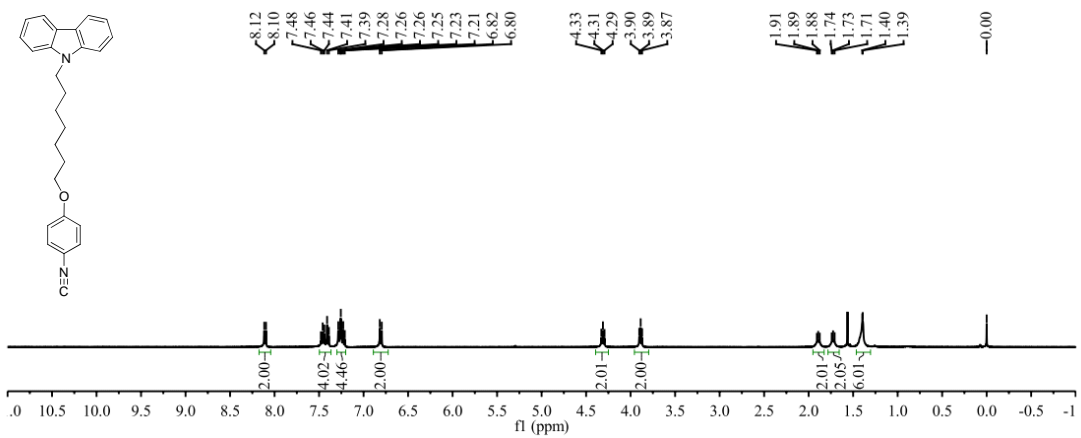
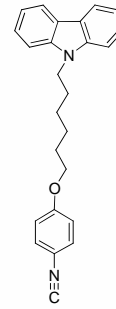
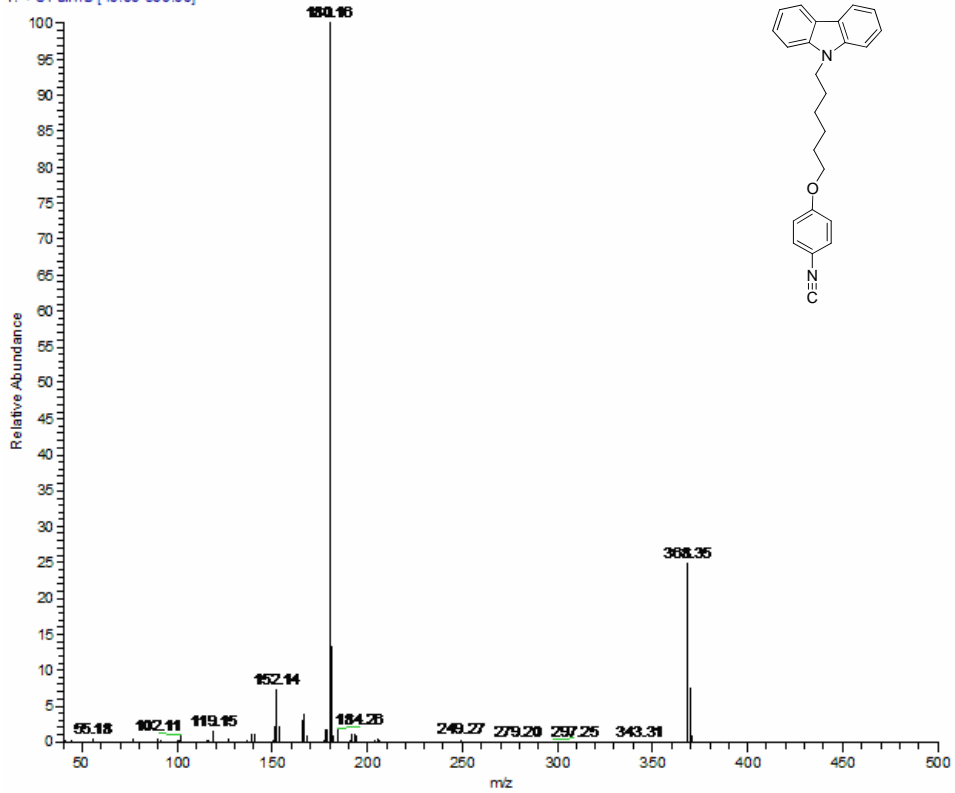
CZ311 #495 RT: 2.32 AV: 1 SB: 552 0.15-2.32, 2.87-3.23 NL: 9.15E5
 T: + cFull.ms [40.00-500.00]



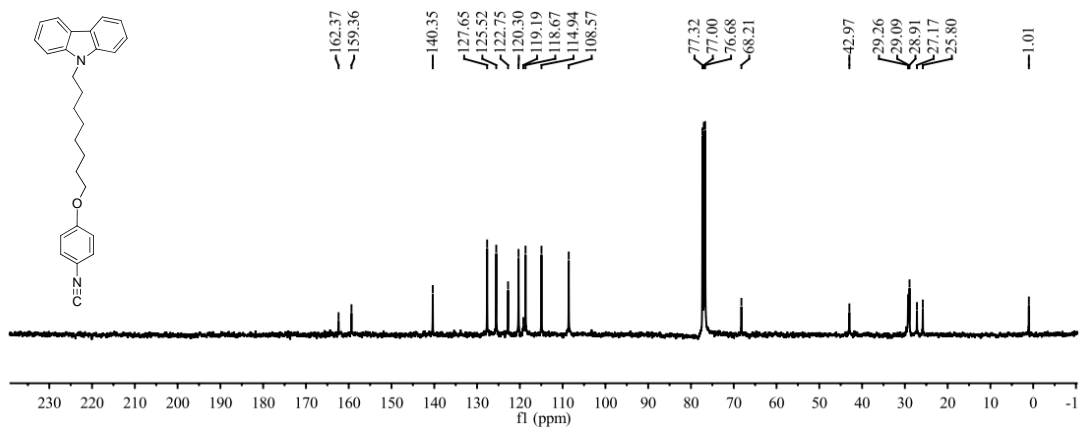
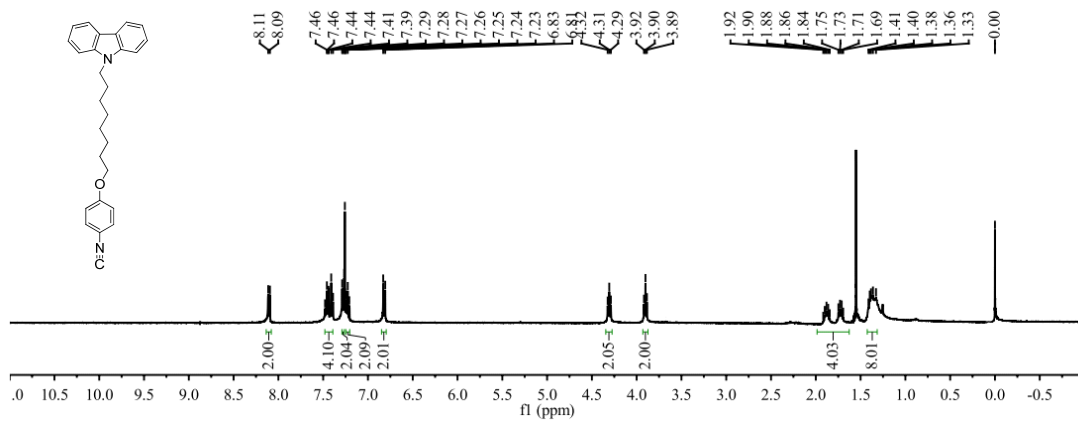
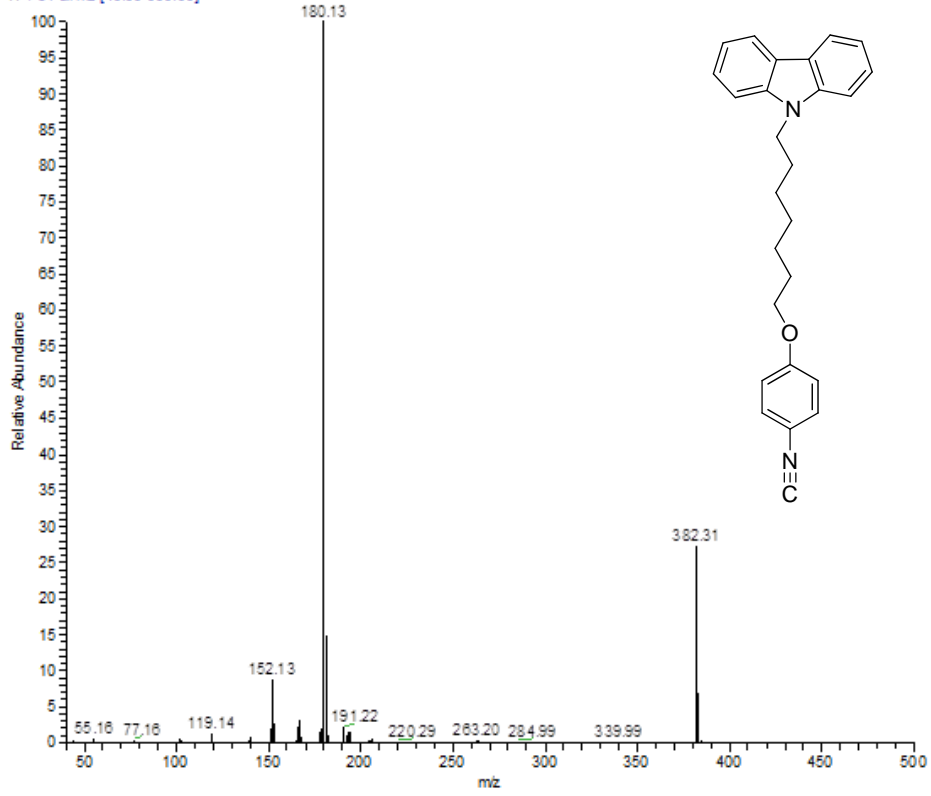
CZ339_141119142745#355 RT: 2.40 AV: 1 SB: 252 0.92-2.18, 2.68-3.08 NL: 1.87E5
 T: + cFull.ms [40.00-500.00]



CZ237 #556 RT: 2.60 AV: 1 SB: 584 0.11-2.33, 2.84-3.30 NL: 123E6
 T: + c Full ms [40.00-500.00]



CZ378 #429 RT: 2.65 AV: 1 SB: 255 1.11-2.32, 2.94-3.22 NL: 1.10E6
 T: + o Full ms [40.00-500.00]



CZ313 #695 RT: 3.24 AV: 1 SB: 512 0.79-2.67, 3.36-3.83 NL: 1.17E7
 T: + cFull.ms [40.00-500.00]

