Rational Design of Gold(I)-NHC Complexes as Anticancer Agents: Induction of Necroptosis and Paraptosis in Lung Adenocarcinoma

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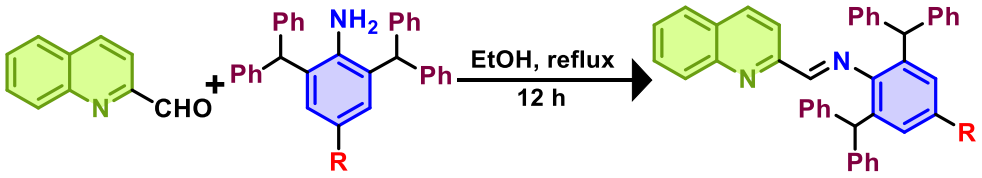
Materials and Instrumentations:

The chemicals and solvents required were purchased from Sigma Aldrich and Merck and were used as received. Anilines were prepared by reported method.[1] DMSO-d^6 were used as solvents for NMR measurements on JEOL 400 and 500 MHz spectrometers. For ^1H and ^{13}C NMR spectroscopy, the chemical shift is reported as dimensionless values and is frequency referenced relative to TMS. Waters Micro mass Quattro Micro triple-quadruplet mass spectrometer was used to collect ESI-MS data. UV–visible spectra were obtained using a JASCO V–670 UV–Visible absorption spectrophotometer. Emission spectra were obtained using Horiba Scientific Fluoromax 4 Spectrofluorometer. FT-IR spectra were recorded on Perkin Elmer Spectrometer in the range of 400-4000 cm-1 using KBr pellets. The following abbreviations are used: m (multiplet), s (singlet), br s (broad singlet), d (doublet), t (triplet) dd (doublet of doublet) and dt (doublet of triplet).

General synthesis of enemines:



Scheme S1: Synthesis of enemines LS1 – LS7

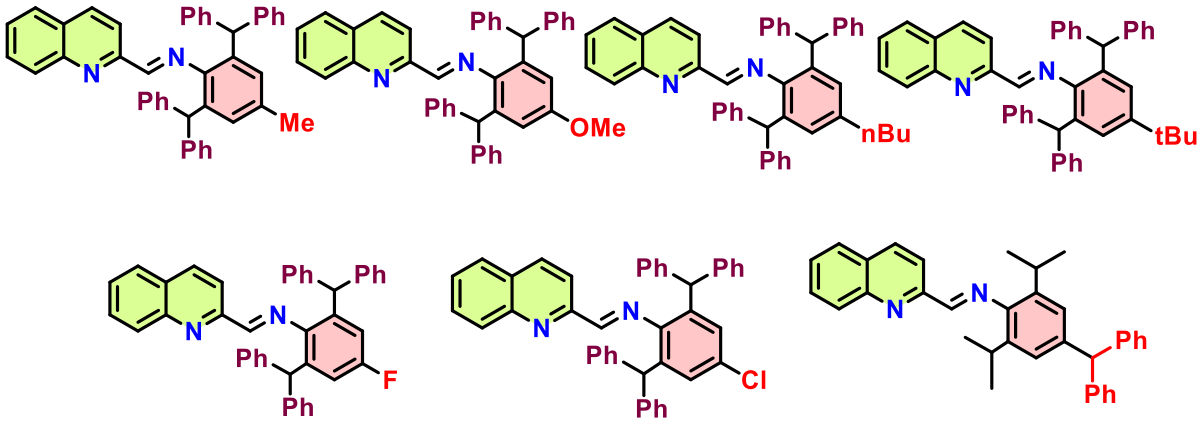
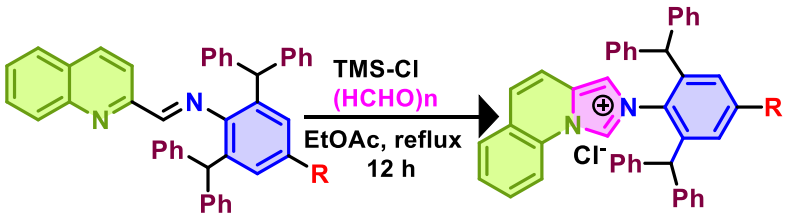


Figure S1: Structure of enemines LS1 – LS7

General synthesis of analogues L1-L7



Scheme S2: Synthesis of analogues L1 – L7

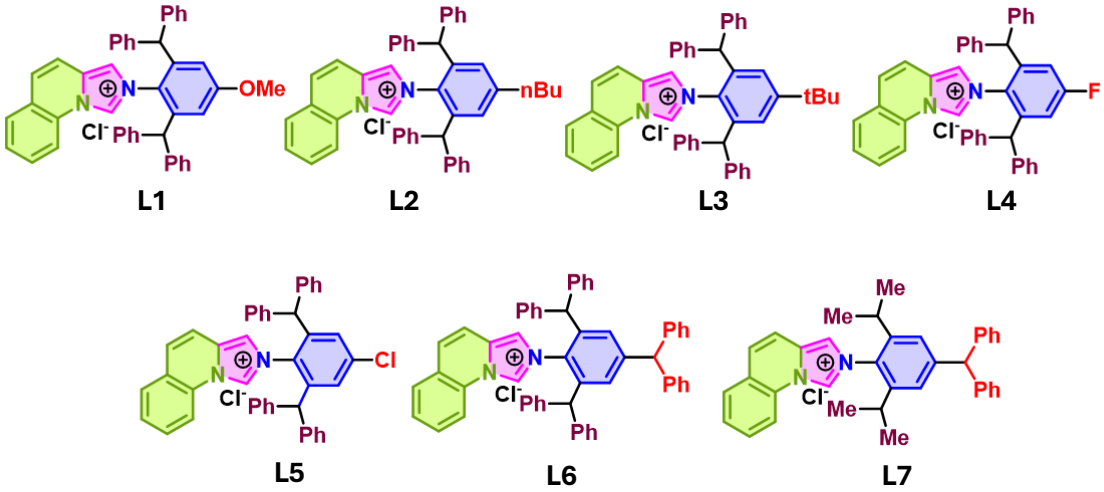
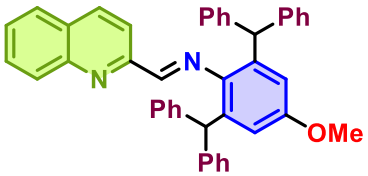


Figure S2: Structure of analogues L1 – L7.

^{1}H NMR and ^{13}C{^{1}H} NMR spectra, ESI spectra of the LS1-LS8

LS1



Yellow solid. Yield: 75%. ^{1}H NMR (δ ppm, DMSO–d_6, 500 MHz): 8.40 (d, J=8.6 Hz, 1H), 8.08 (d, J=8.6, 1H), 7.99 (d, J=8.1 Hz, 1H), 7.91 (d, J=8.4 Hz, 1H), 7.75 (t, J= 7.0 Hz, 1H), 7.67-7.59 (m, 1H), 7.40 (s, 1H), 7.16 (dt, J=28.5, 7.4 Hz, 12H), 6.97 (d, J=7.2 Hz,8H), 6.33 (s, 2H), 5.44(s, 2H), 3.44 (s, 3H). ^{13}C NMR (δ ppm DMSO–d_6, 100 MHz, proton decoupled): 165.91,155.81,155.65,154.20,143.68,143.48,134.68,130.58,129.81,129.85,128.84,128.44,126.87,118.40,113.85,56.29,52.07. ESI-MS (ES^{+}; [M+H]$^{+}$ m/z) calculated for $C_{43}H_{35}N_2O$: 595.2749, observed : 595.2744.

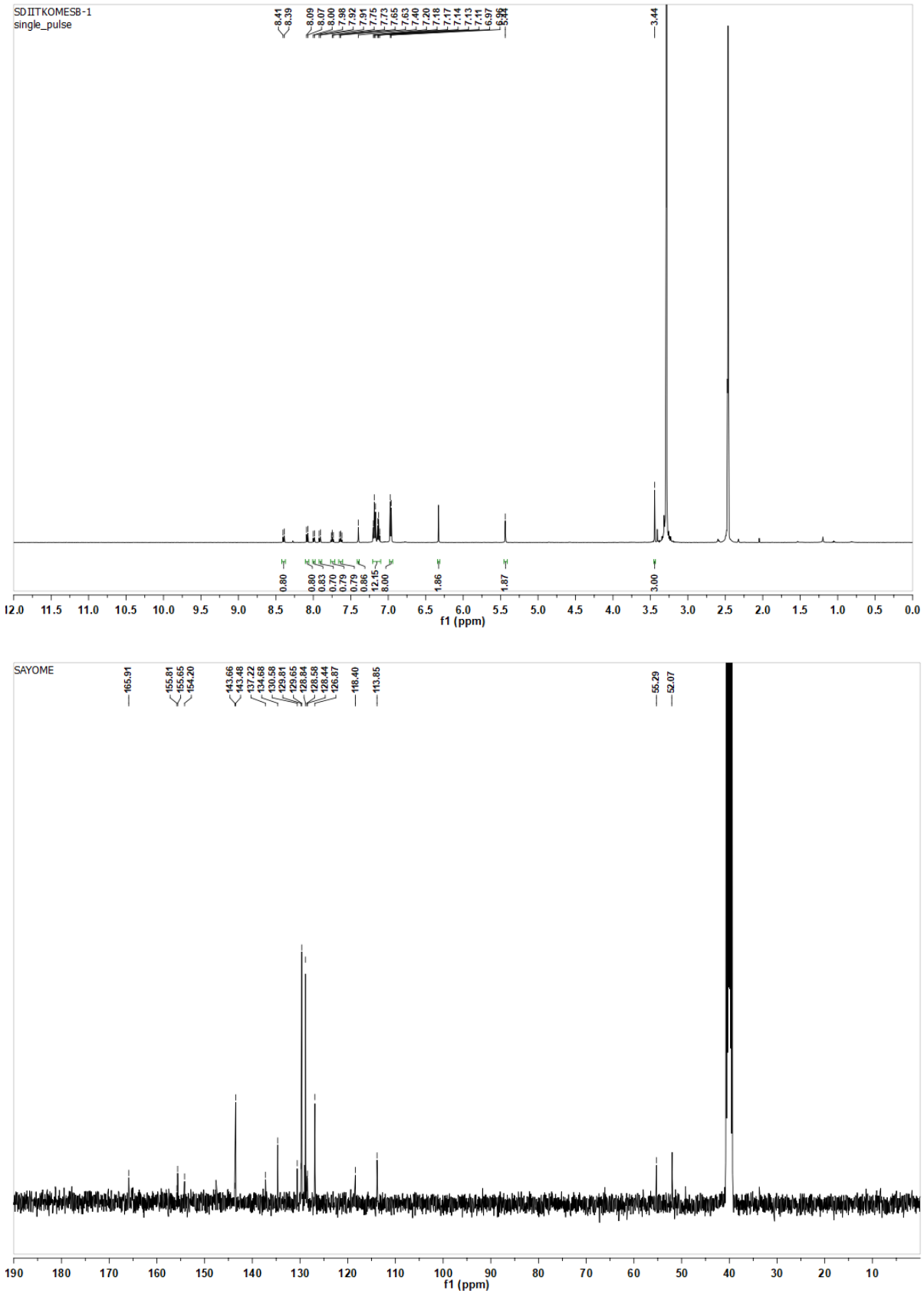
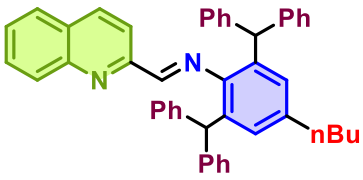
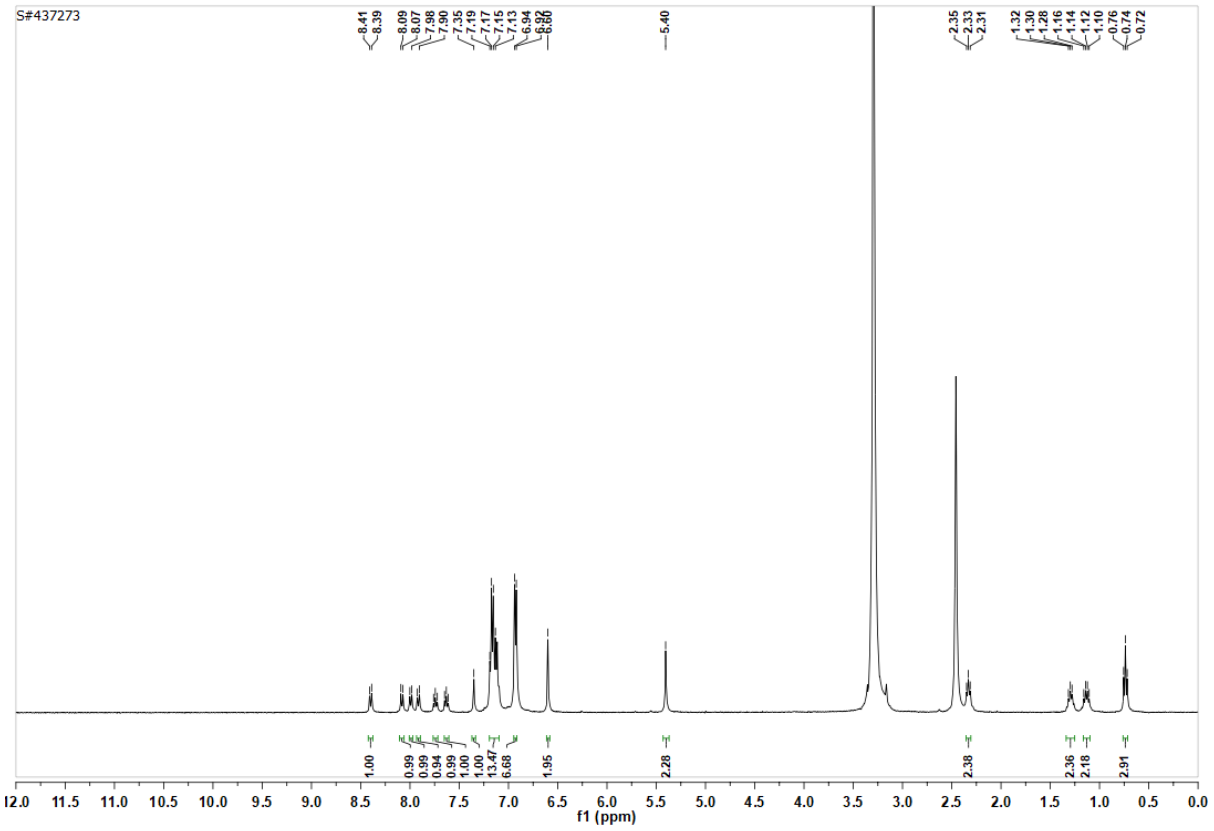


Figure S3. ^{1}H NMR and $^{13}C\{^{1}H\}$ NMR spectra of the LS1

LS2



Yellow solid. Yield: 80%. ^{1}H NMR (δ ppm, DMSO–d_6, 500 MHz): ^{1}H NMR (400 MHz, DMSO-D6) δ 8.40 (d, J = 8.5 Hz, 1H), 8.08 (d, J = 8.6 Hz, 1H), 7.99 (d, J = 8.0 Hz, 1H), 7.91 (d, J = 8.4 Hz, 1H), 7.74 (t, J = 7.6 Hz, 1H), 7.63 (t, J = 7.3 Hz, 1H), 7.35 (s, 1H), 7.16 (m, J =13H), 6.93 (d, J = 7.1 Hz, 7H), 6.60 (s, 2H), 5.40 (s, 2H), 2.33 (t, J = 7.3 Hz, 2H), 1.34 – 1.25 (m, 2H), 1.13 (dd, J = 14.6, 7.3 Hz, 2H), 0.74 (t, J = 7.3 Hz, 3H). ^{13}C NMR (δ ppm DMSO–d_6, 100 MHz, proton decoupled):154.17,143.34,137.26, 129.83,129.65,128.79,128.55,128.10, 126.79, 51.68,34.92, 33.50,21.85,13.28. ESI-MS (ES+;[M+H]$^{+}$ m/z) calculated for $C_{46}H_{41}N_2$: 621.3269, observed 621.3268.



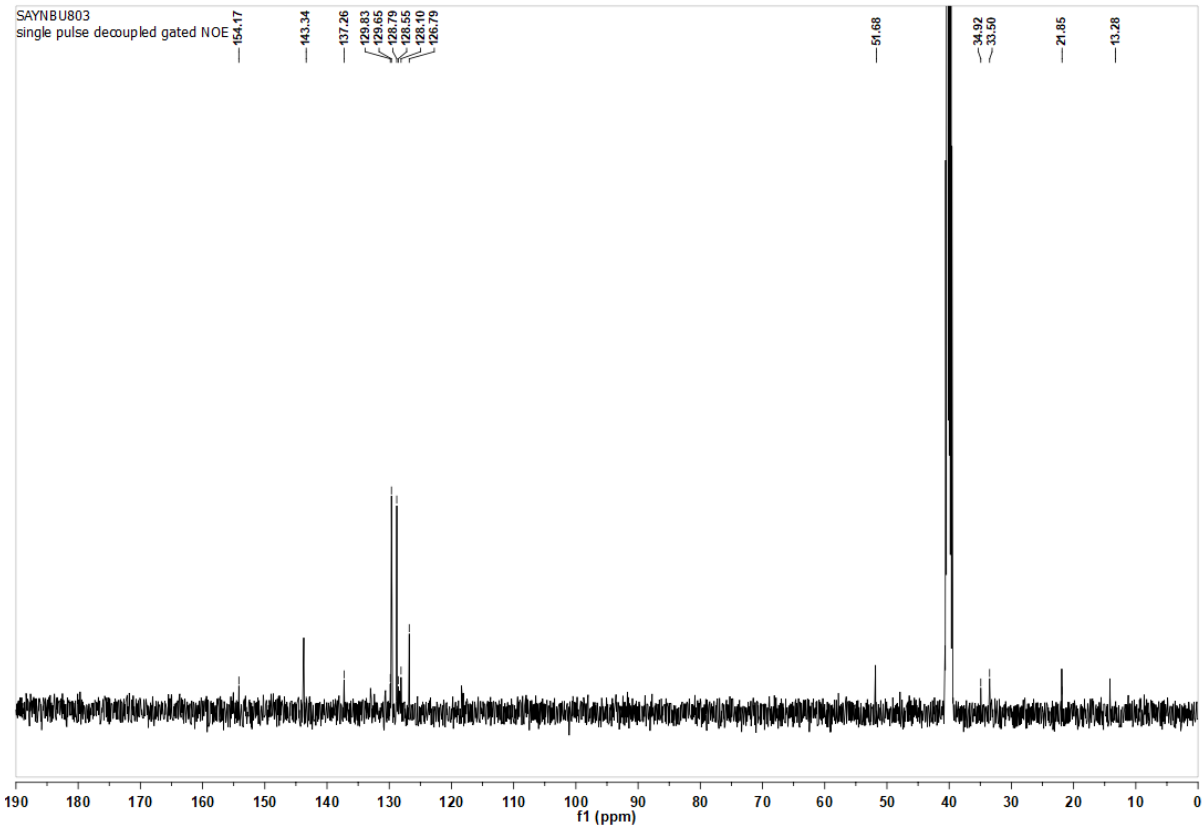
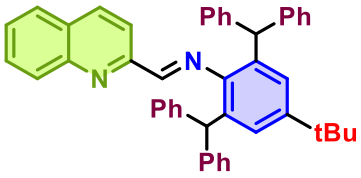


Figure S4. ^{1}H NMR and ^{13}C{^{1}H} NMR spectra of the LS2

LS3



Yellow solid. Yield: 71%. ^{1}H NMR (δ ppm, DMSO–d_6, 500 MHz): 8.37 (d, J= 8.6 Hz, 1H), 8.05 (d, J=8.5, 1H), 8.00 (d, J=15.6, 8.3 Hz, 2H), 7.92 (d, J=8.4 Hz, 1H), 7.73 (t, J= 7.6 Hz, 1H), 7.62 (t, J=7.75 Hz, 1H), 7.39 (s, 1H), 7.19-7.09 (m, 12H), 6.93 (d,7.3 Hz, 8H), 6.80 (s, 2H), 5.41 (s, 2H) 0.98 (s, 9H). ^{13}C NMR (δ ppm DMSO–d_6, 100 MHz, proton decoupled): 165.27, 154.15, 147.61, 145.30, 143,57, 137.29, 132.47, 129.61, 128.75, 126.77, 125.03, 118.51, 52.12, 34.46, 31.51. ESI-MS (ES+;[M+H]$^{+}$ m/z) calculated for $C_{46}H_{41}N_2$: 621.3269,observed 621.3269.

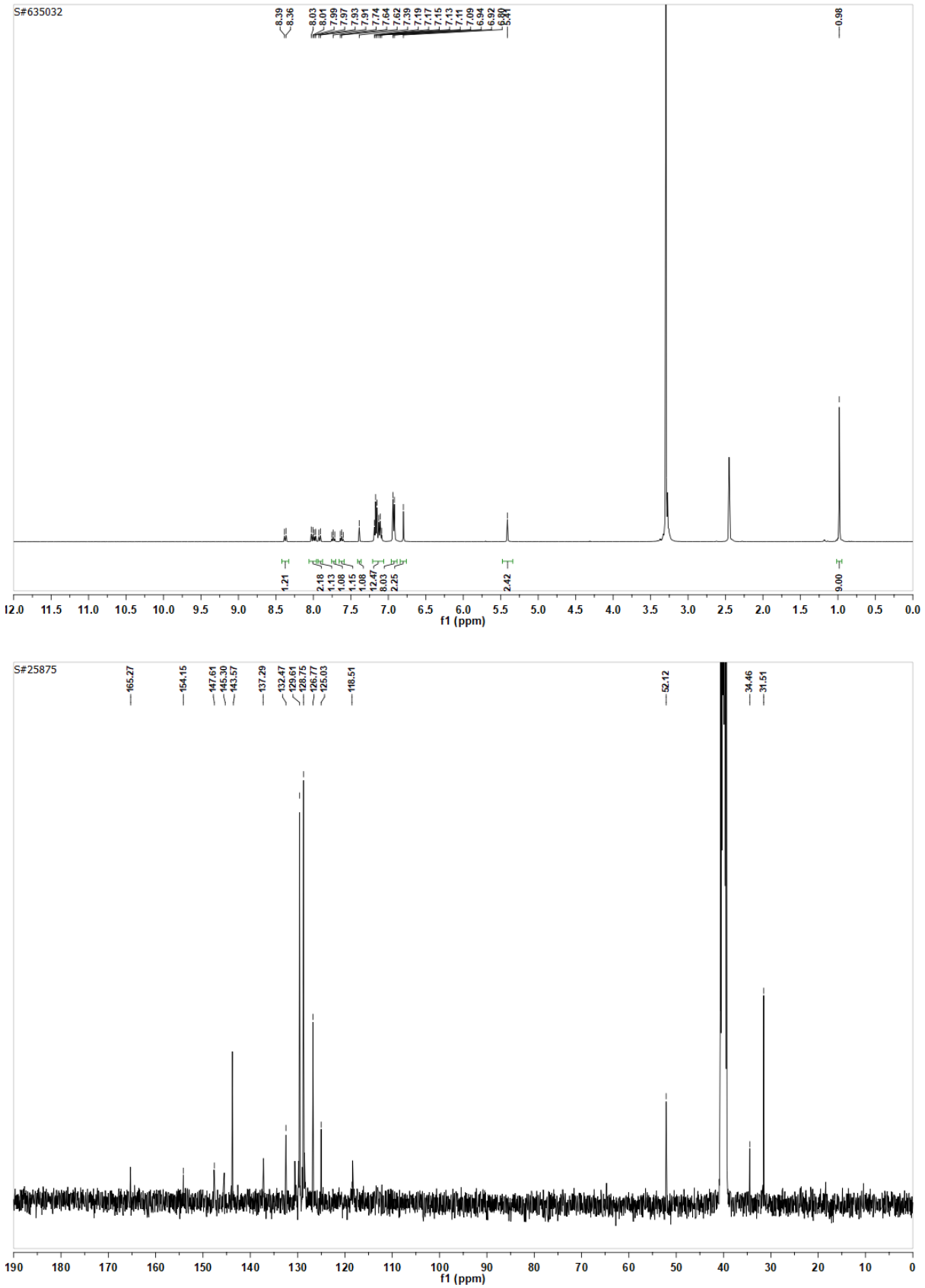
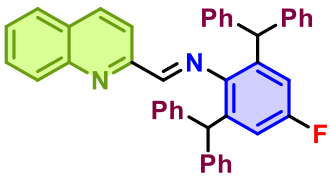
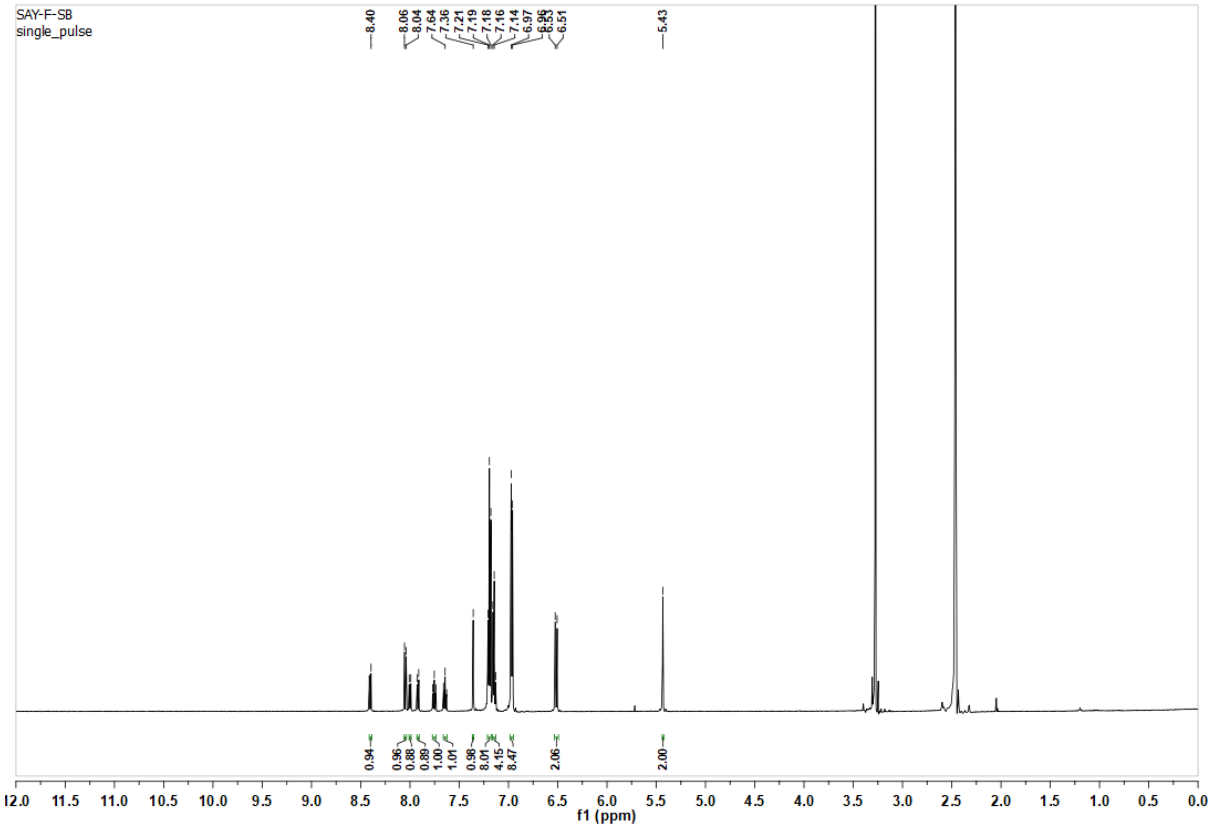


Figure S5. ^{1}H NMR and $^{13}C\{^{1}H\}$ NMR spectra of the LS3

LS4



Yellowish White solid. Yield: 76%. ^{1}H NMR (δ ppm, DMSO–d_6, 500 MHz): 8.40 (d, 1H), 8.05 (d, J=8.5, 1H), 8.00 (d, J=8.1 Hz, 1H), 7.92 (d, J=8.4 Hz, 1H), 7.75 (t, J= 8.3 Hz, 1H), 7.64 (t, J=8.1 Hz, 1H), 7.36 (s, 1H), 7.21-7.14 (m, 12H), 6.97-6.96 (m,8H), 6.52 (d, J=9.7 Hz, 2H), 5.43(s, 2H). ^{13}C NMR (δ ppm DMSO–d_6, 100 MHz, proton decoupled): 166.50, 157.87, 153.83, 147.61, 137.28, 135.67, 130.64, 129.85, 129.63, 129.08, 128.97, 128.55, 127.08, 118.40, 114.88, 114.69, 51.97. ESI-MS (ES+;[M+H]$^{+}$ m/z) calculated for $C_{42}H_{32}FN_2$: 583.2549, observed 583.2538.



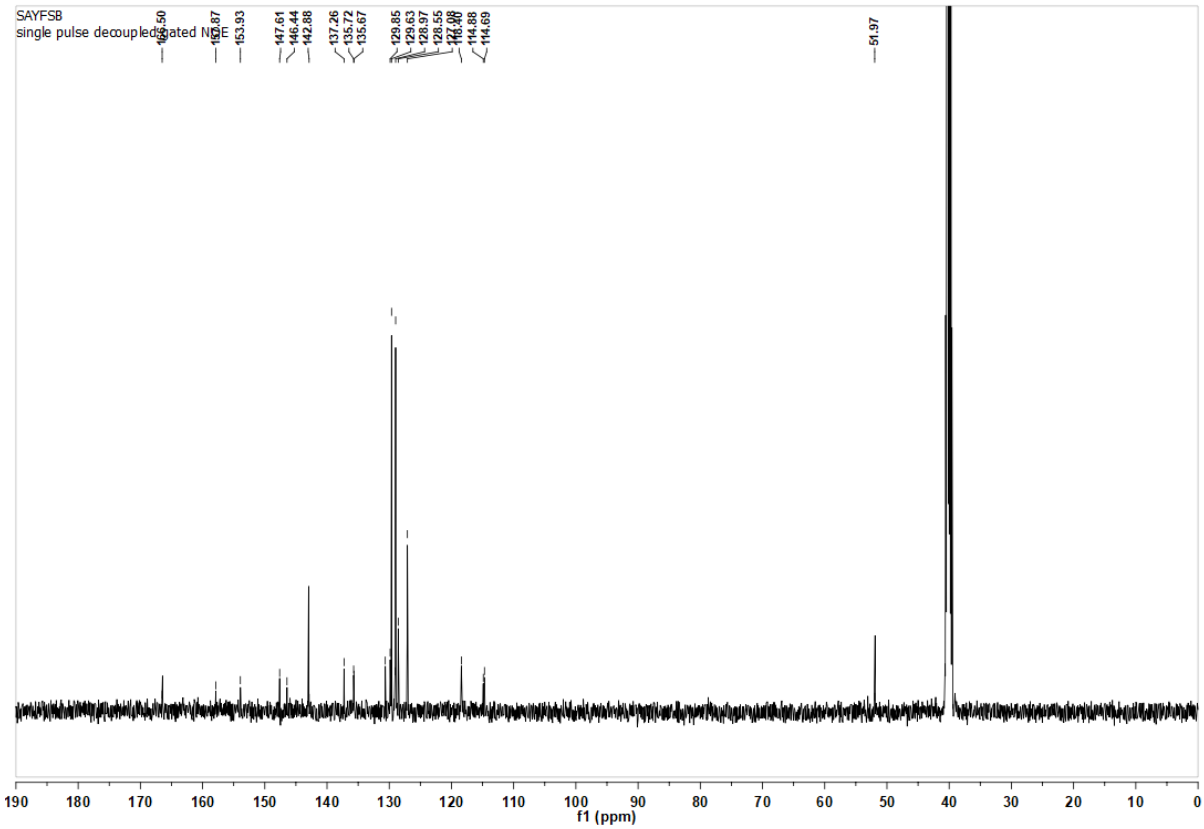
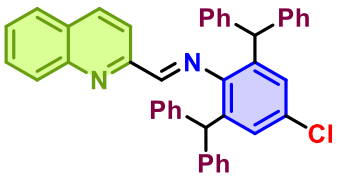


Figure S6. ^{1}H NMR and ^{13}C{^{1}H} NMR spectra of the LS4

LS5



Yellowish white solid. Yield: 79%. ^{1}H NMR (δ ppm, DMSO–d_6, 500 MHz): δ 8.45 (d, J = 8.7 Hz, 1H), 8.07 – 8.03 (m, 1H), 7.97 (d, J = 8.6 Hz, 1H), 7.80 (t, J = 7.1 Hz,1H), 7.70 (t, J = 7.5 Hz, 1H), 7.38 (s, 1H), 7.32 (t, J = 7.6 Hz,1H), 7.22 (m,7.25-7.23, 8H), 7.06 (m,7.21-7.18, 4H), 7.00 (d, J = 7.1Hz, 5H), 6.76 (s, 2H), 5.47 (s, 2H).^{13}C NMR (δ ppm DMSO–d_6, 100 MHz, proton decoupled): 166.21, 142.79, 137.28, 135.75, 130.67, 129.85,129.65, 129.09, 128.61, 128.55, 128.10, 127.79, 127.61, 127.13, 127.08, 118.32, 51.83. ESI-MS (ES+;[M+H]$^{+}$ m/z) calculated for $C_{42}H_{32}ClN_2$: 599.2254, observed 599.2255.

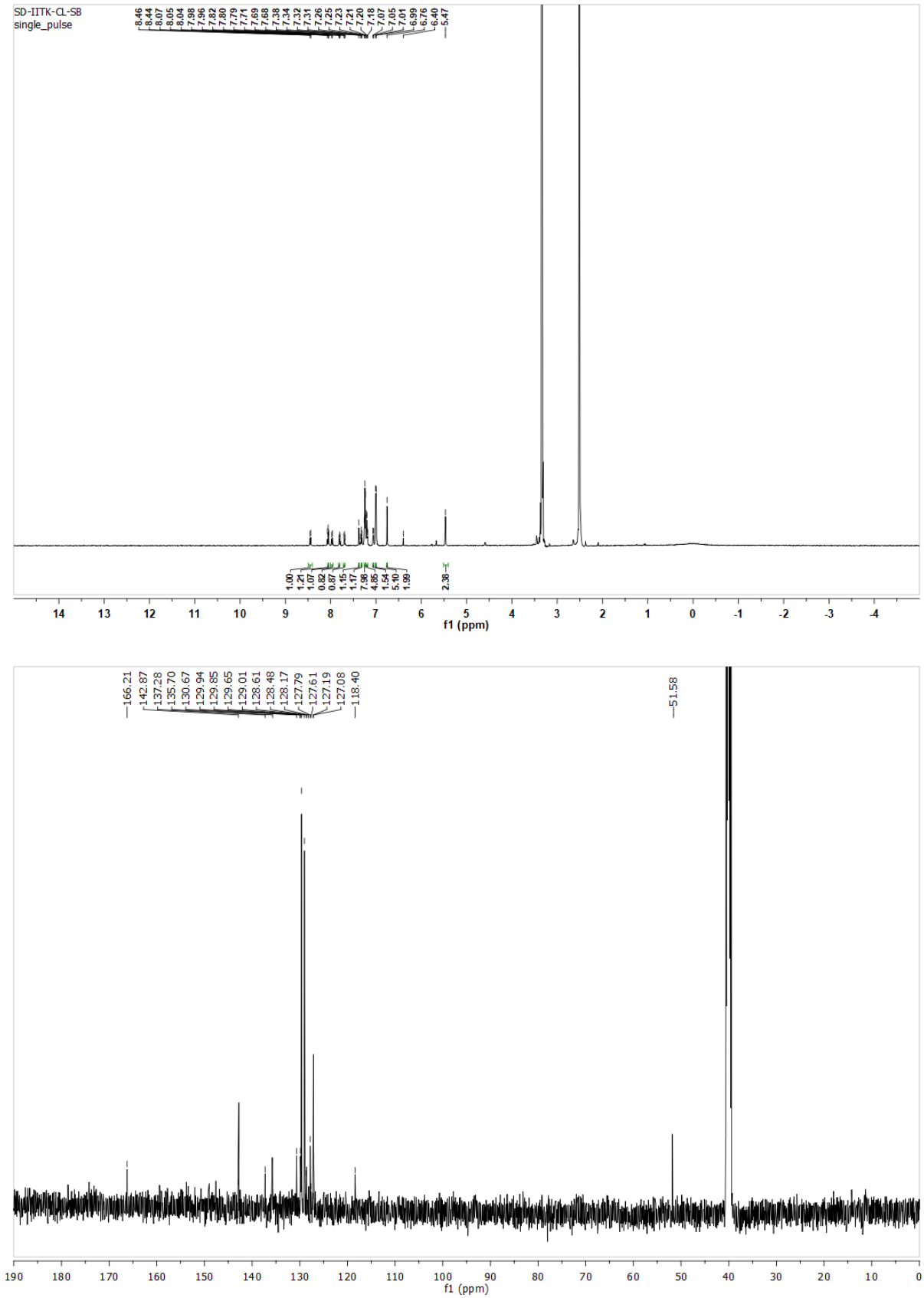
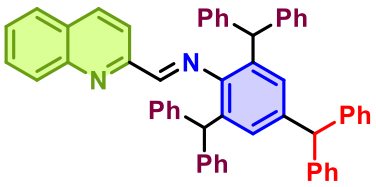
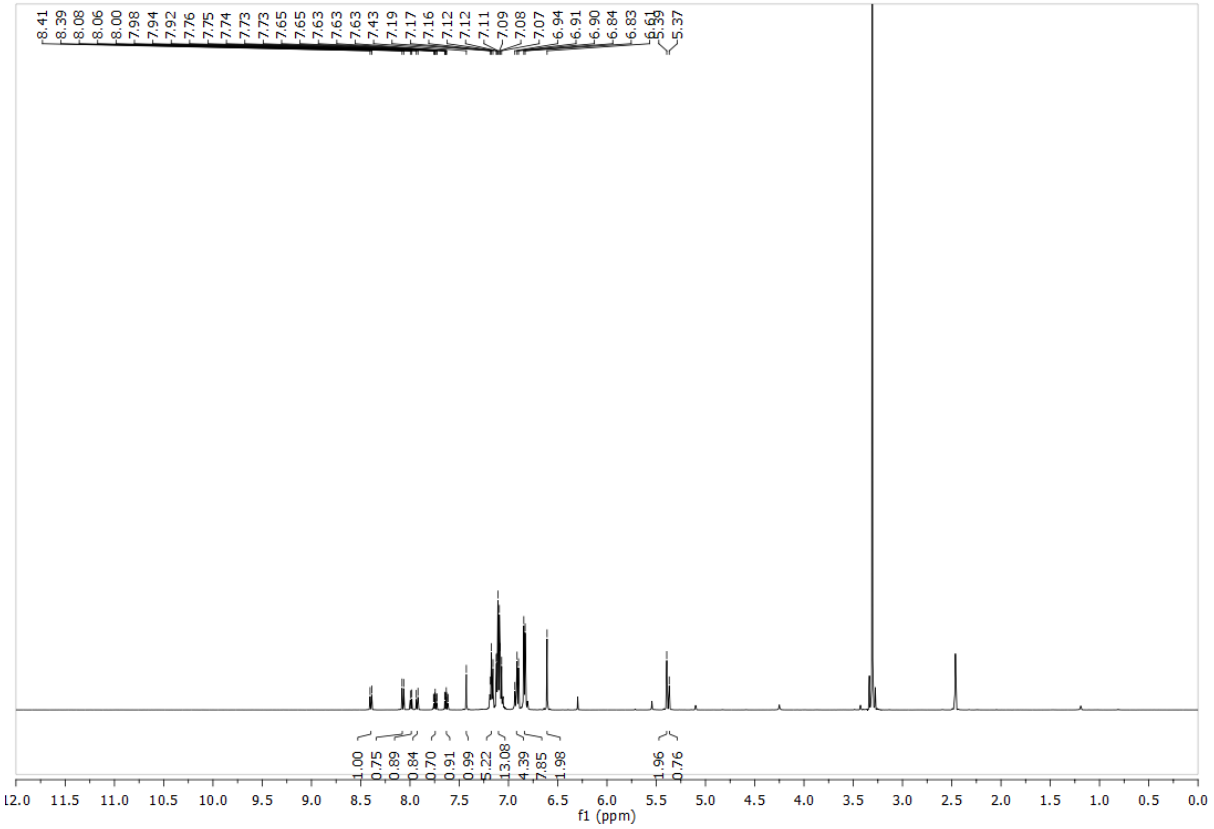


Figure S7. ^{1}H NMR and $^{13}C\{^{1}H\}$ NMR spectra of the LS5

LS6



Yellowish white solid. Yield: 83%. ^{1}H NMR (δ ppm, DMSO–d_6, 500 MHz): δ 8.40 (d, J = 8.7 Hz, 1H), 8.07 (d, J = 8.6 Hz, 1H), 7.99 (d, J = 7.3 Hz, 1H), 7.93 (d, J = 8.5 Hz, 1H), 7.74 (ddd, J = 8.4, 6.9, 1.4 Hz, 1H), 7.63 (ddd, J = 8.1, 6.9, 1.1 Hz, 1H), 7.43 (s, 1H), 7.19-7.16 (m, 5H), 7.13 – 7.04 (m, 13H), 6.94-6.90 (m, 4H), 6.84 (d, J = 6.8 Hz, 8H), 6.61 (s, 2H), 5.39 (s, 1H), 5.37 (s, 1H). ^{13}C NMR (δ ppm DMSO–d_6, 100 MHz, proton decoupled):165.47,154.09,144.45, 143.58, 132.88, 129.55, 129.47, 129.32, 129.27, 128.72, 128.68, 126.73, 126.60, 118.40, 55.64, 51.79.ESI-MS (ES+;[M+H]$^{+}$ m/z) calculated for $C_{55}H_{43}N_2$: 731.3246, observed: 731.3433.



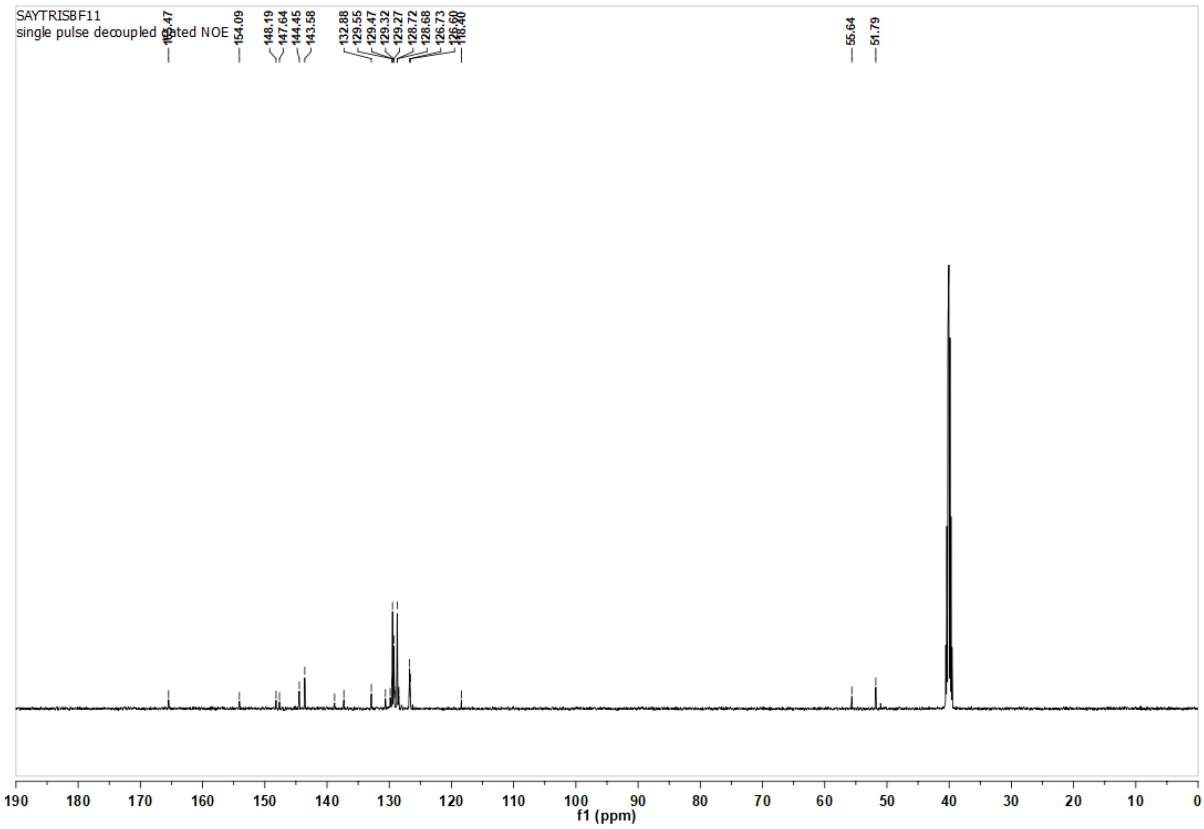
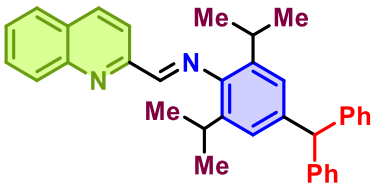


Figure S8. ^{1}H NMR and $^{13}C\{^{1}H\}$ NMR spectra of the LS6

LS7



NMR (500 MHz,) δ 8.51 (d, *J* = 8.6 Hz,1H), 8.40 (s,1H), 8.29 (d, *J* = 8.5 Hz,1H), 8.11 (d, *J* = 8.0 Hz,1H), 8.05 (d, *J* = 7.3 Hz,1H), 7.82 (ddd, *J* = 8.4, 6.9, 1.4 Hz,1H), 7.68 (ddd, *J* = 8.1, 7.0, 1.1 Hz,1H), 7.33-7.28 (m, 5H), 7.21-7.16 (m, 2H), 7.16 – 7.12 (m, 4H), 6.93 (s,2H), 5.57 (s, 1H), 2.85 (m, 2H), 1.00 (d, *J* = 6.9 Hz, 12 H). ^{13}C NMR (*δ* ppm DMSO–d_6, 100 MHz, proton decoupled): 164.02,154.42, 147.85, 146.64,144.75, 140.04, 137.96, 136.87, 130.94, 129.80, 129.52, 128.84,128.70, 126.72, 124.31, 118.36, 56.29, 28.09, 23.75.ESI-MS (ES+;$[M+H]^+$ m/z) calculated for $C_{35}H_{35}N_2$: 483.2800 , observed: 483.2813.

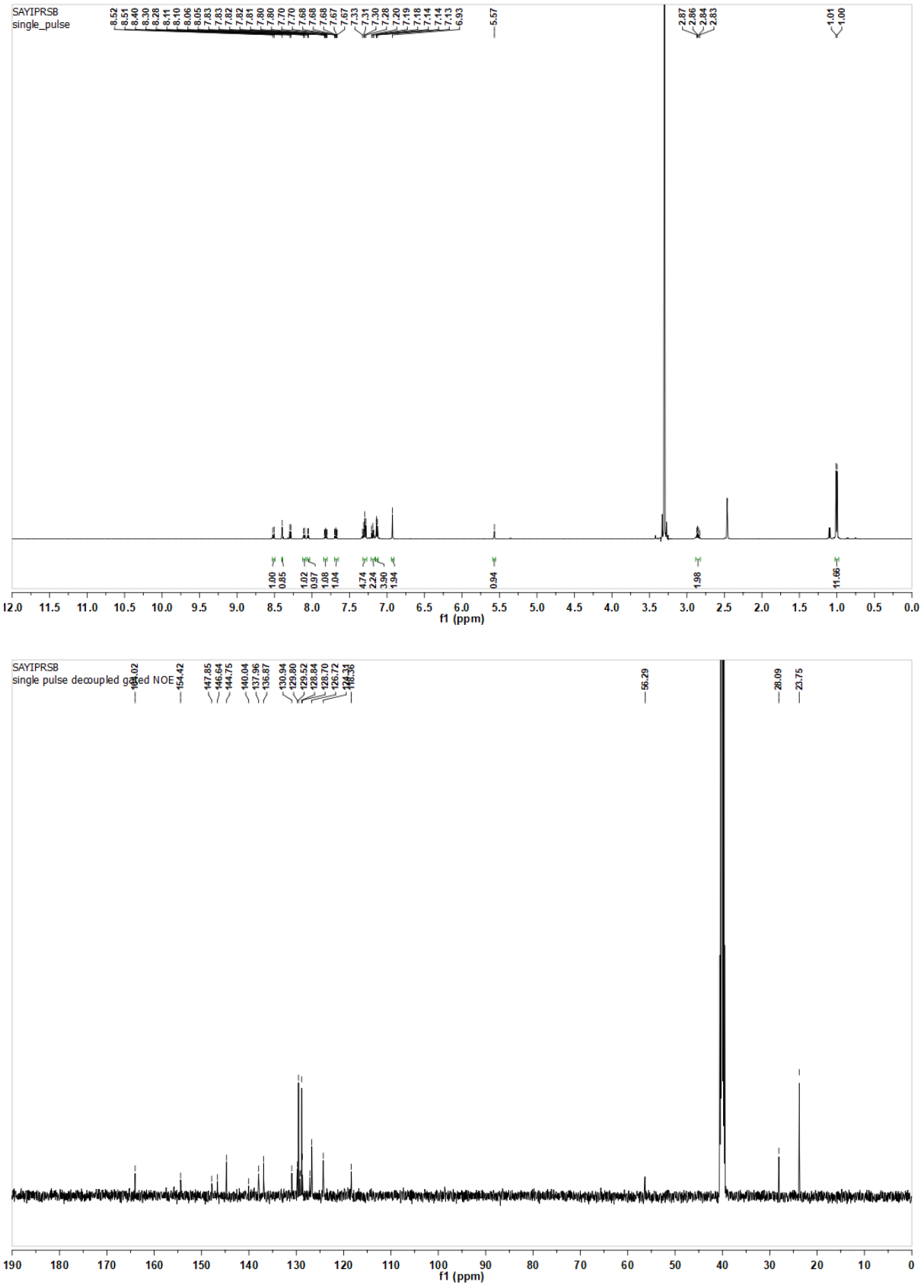
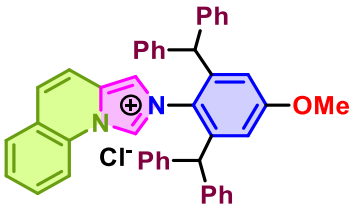
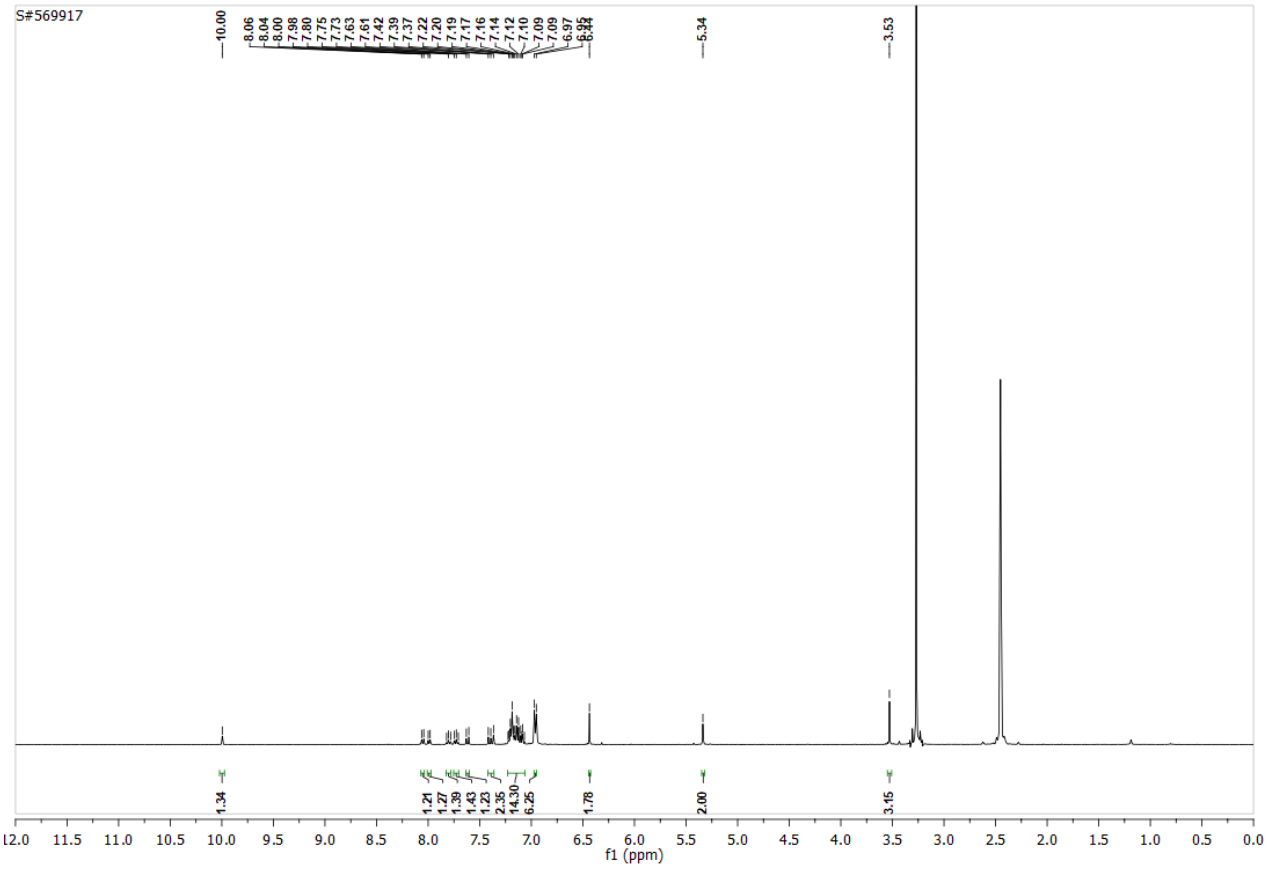


Figure S9. ^{1}H NMR and $^{13}C\{^{1}H\}$ NMR spectra of the LS7

L1



White solid. Yield: 82%. ^{1}H NMR (δ ppm, DMSO–d_6, 400 MHz): 10.00 (s, 1H), 8.05 (d, J=8.2, 1H), 7.99 (d, J=7.7 Hz, 1H), 7.80 (t, J=7.8 Hz, 1H), 7.73 (t, J= 7.6 Hz, 1H), 7.62 (d, 9.7 Hz, 1H), 7.43-7.35 (m, 2H), 7.223-7.07 (m, 14H), 6.97-6.92(m, 6H), 6.44 (s, 2H), 5.34(s, 2H), 3.53 (s, 3H). ^{13}C NMR (δ ppm DMSO–d_6, 100 MHz, proton decoupled): 160.50, 143.80, 141.90, 130.53, 130.01, 129.42, 129.07, 128.29, 127.45, 126.68, 124.73, 117.85, 115.45, 114.80, 55.07, 51.54. ESI-MS (ES+;[M]$^{+}$ m/z) calculated for $C_{44}H_{33}N_2O^{+}$:607.2743, observed: 607.2732.



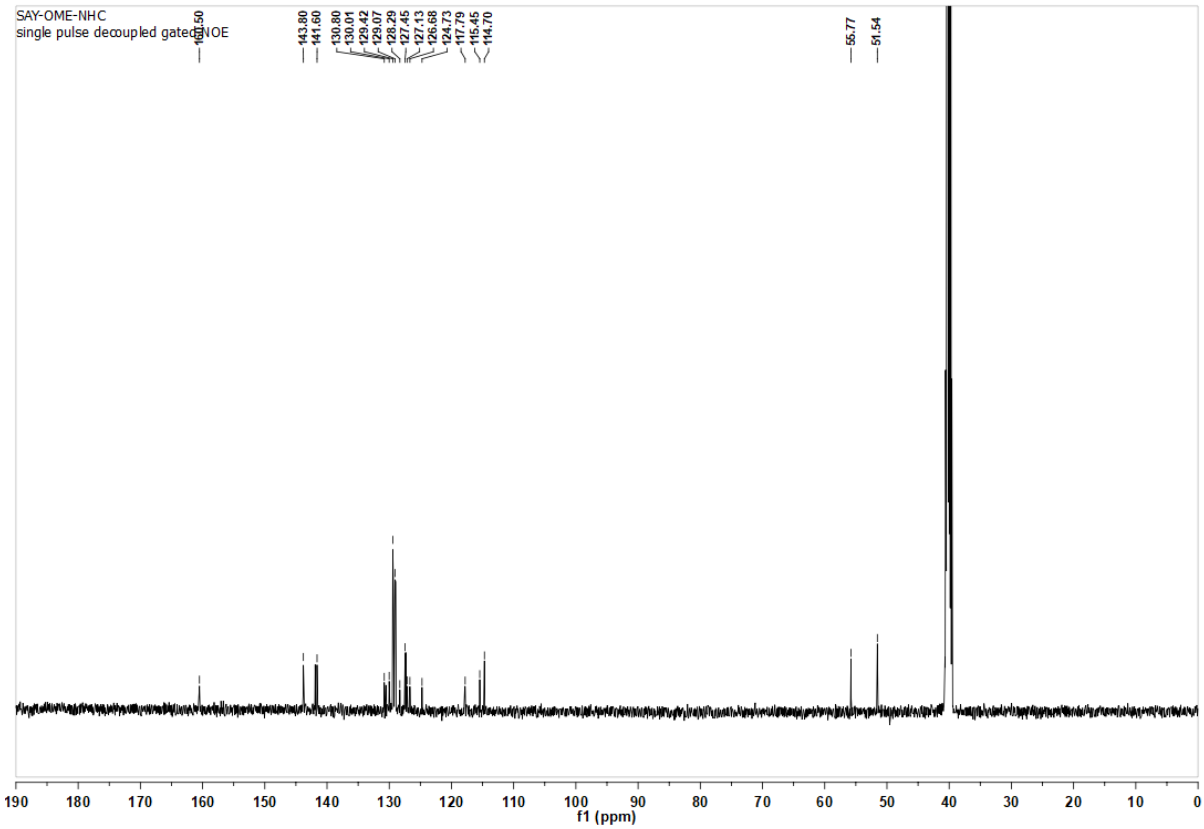
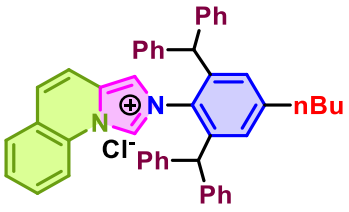
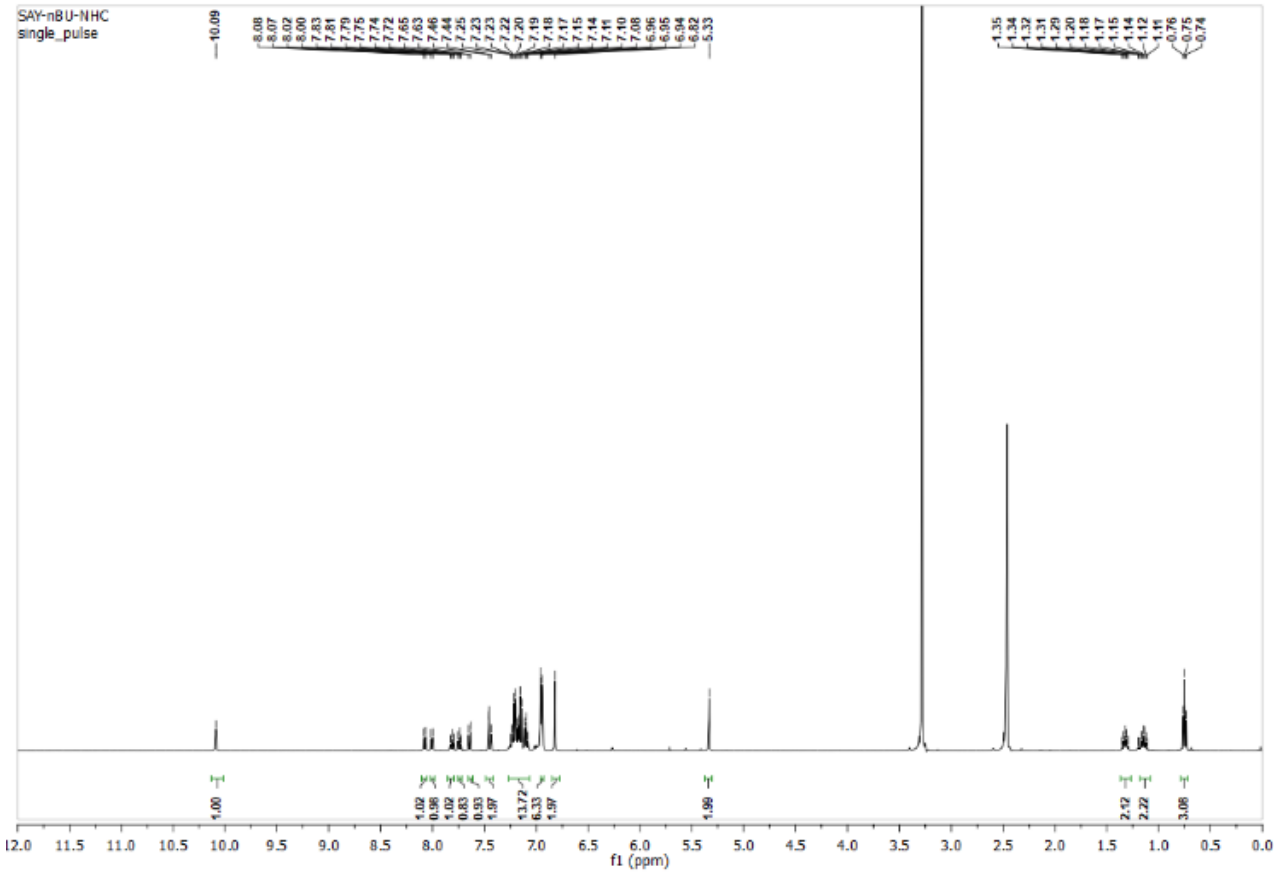


Figure S10. ^{1}H NMR and $^{13}C\{^{1}H\}$ NMR spectra of L1

L2



White solid. Yield: 88%. ^{1}H NMR (δ ppm, DMSO–d_6, 500 MHz): 10.09 (s, 1H), 8.08 (d, J=8.3, 1H), 8.01 (d, J=9.0 Hz, 1H), 7.81 (t, J=7.8 Hz, 1H), 7.74 (t, J= 7.6 Hz, 1H), 7.64 (d, 9.7 Hz, 1H), 7.45 (d, J=11.1 Hz, 2H) 7.25-7.06 (m, 14H), 6.98-6.92(m, 6H), 6.82 (s, 2H), 5.33 (s, 2H),2.49-2.47 (m, 2H) 1.32 (dt, J= 15.0, 7.5 Hz, 2H), 1.22-1.07 (m, 2H), 0.75 (t, J=7.5 Hz, 2H). ^{13}C NMR (δ ppm DMSO–d_6, 100 MHz, proton decoupled): 145.59, 142.18, 131.61, 130.56, 130.40, 130.04, 129.43, 128.94, 128.56, 127.40, 124.79, 117.54, 115.53, 51.28, 35.02, 33.07, 21.74, 14.08. ESI-MS (ES+;[M]$^{+}$ m/z) calculated for $C_{47}H_{41}N_2^{+}$:633.3264, observed: 633.3264.



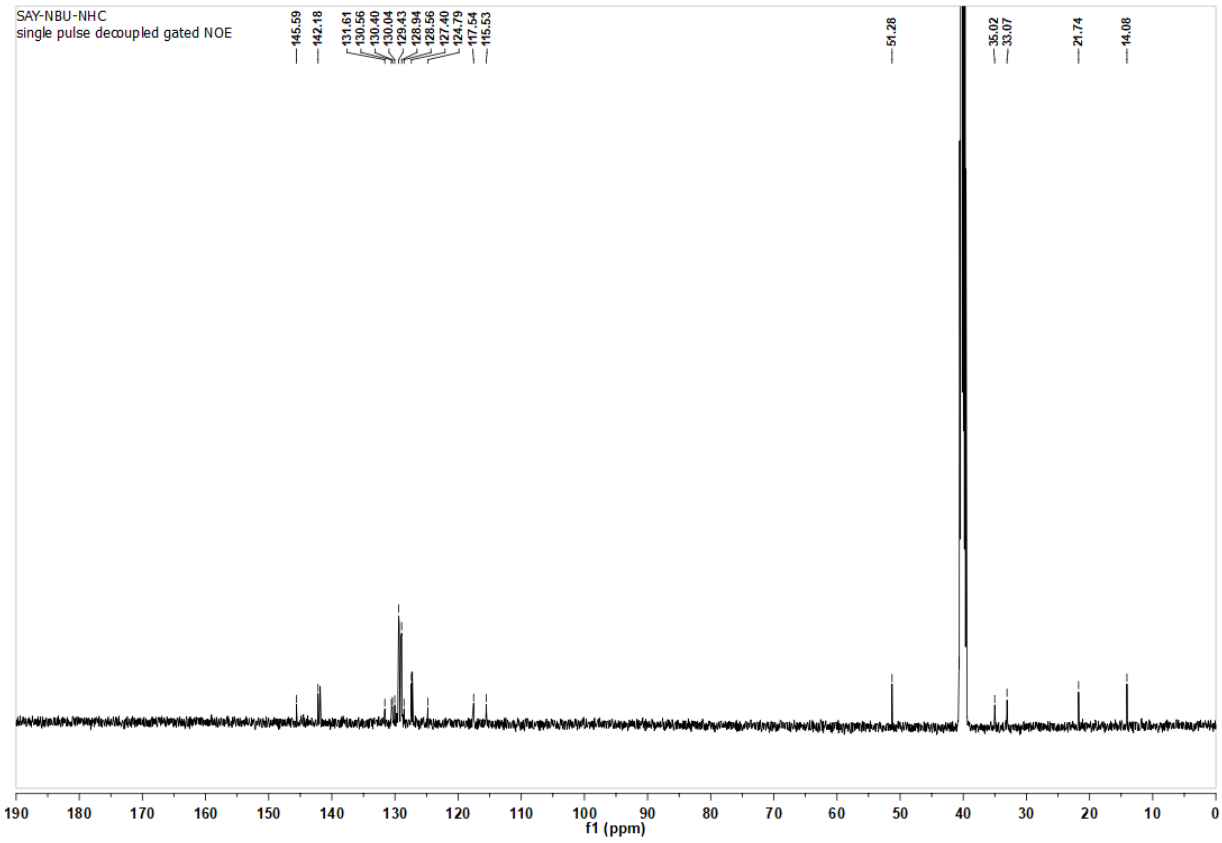
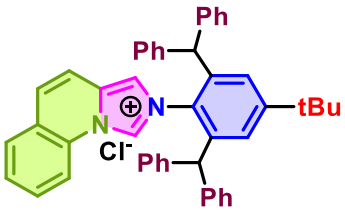
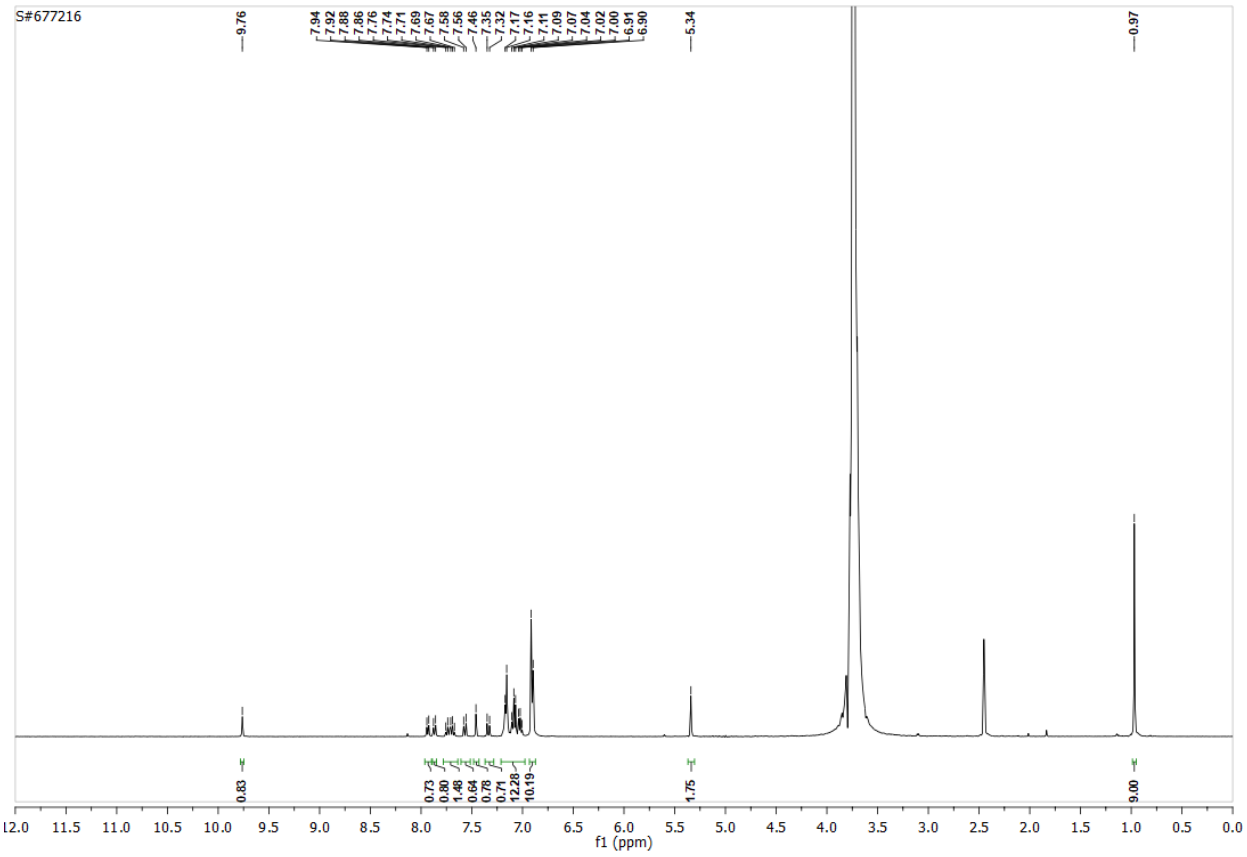


Figure S11. ^{1}H NMR and $^{13}C\{^{1}H\}$ NMR spectra of L2

L3



White solid. Yield: 80%. ^{1}H NMR (δ ppm, DMSO–d_6, 500 MHz): 9.76 (s, 1H), 7.93 (d, J=7.6 Hz, 1H), 7.87 (d, J=8.2 Hz, 1H), 7.71 (m, 1H), 7.57 (d, 9.6 Hz, 1H), 7.46 (s, 1H), 7.37 (d, J=9.7 Hz, 1H), 7.24-6.98 (m, 12H), 6.90(d, J=7.5 Hz, 10H), 5.34(s, 2H), 0.97 (s, 4H), ^{13}C NMR (δ ppm DMSO–d_6, 100 MHz, proton decoupled):153.22,142.04,141.85,141.49,129.39.129.05,128.88,127.37,127.21,17.92,117.44 ,115.38,51.71,35.15,31.05. ESI-MS (ES+; $[M]^+$ m/z) calculated for $C_{47}H_{41}N_2^+$:633.3264, observed: 633.3264.



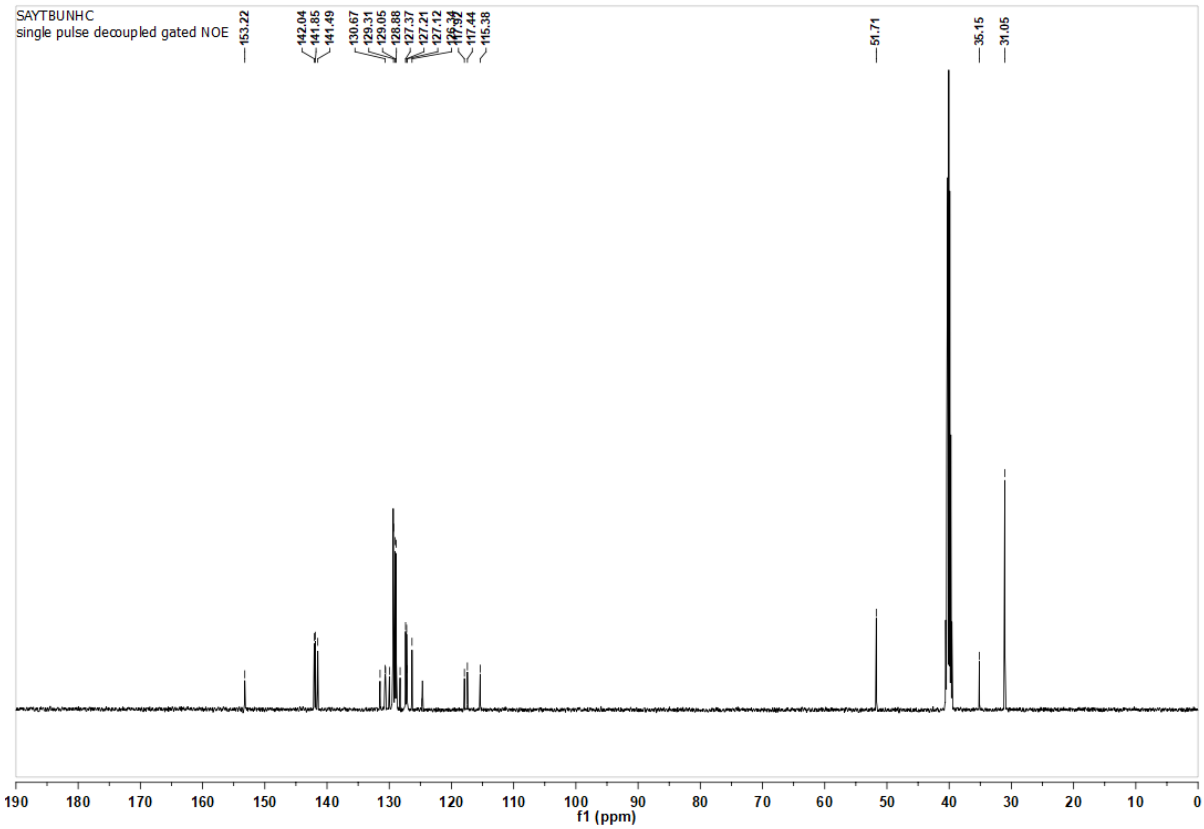
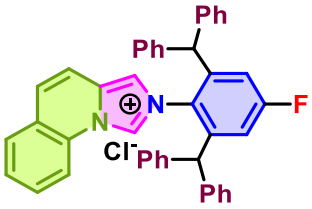
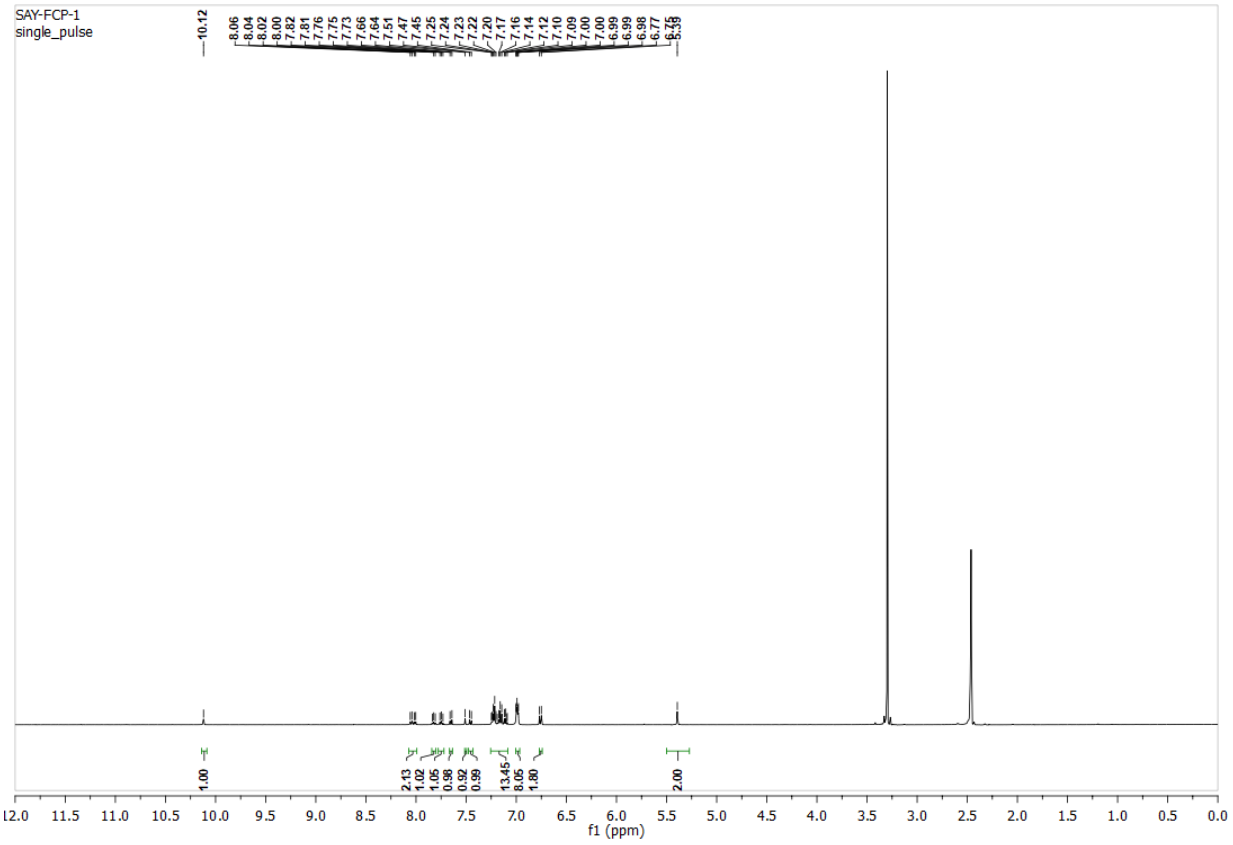


Figure S12. ^{1}H NMR and $^{13}C\{^{1}H\}$ NMR spectra of L3

L4



White solid. Yield: 82%. ^{1}H NMR (δ ppm, DMSO–d_6, 500 MHz): 10.12 (s, 1H), 8.03 (dd, J=19.6,8.0 Hz, 2H), 7.82 (t, J=7.4 Hz, 1H), 7.75 (t, J= 7.7 Hz, 1H), 7.65 (d, 9.6 Hz, 1H), 7.51 (s, 1H), 7.46 (d, J=9.7 Hz, 1H), 7.26-7.06 (m, 13H), 7.02-6.94(m, 8H), 6.76 (d, J=9.2 Hz, 2H), 5.39(s, 2H). ^{13}C NMR (δ ppm DMSO–d_6, 100 MHz, proton decoupled):163.77, 161.76, 145.53, 141.41, 141.13, 130.89, 130.58, 130.03, 129.49, 129.42, 129.34, 129.19, 129.06, 128.40, 127.61, 127.44, 127.25, 124.71, 117.98, 117.42, 116.44, 116.25, 115.40, 51.46. ESI-MS (ES+; $[M]^+$ m/z) calculated for $C_{43}H_{32}FN_2^+$: 595.2544, observed: 595.2532.



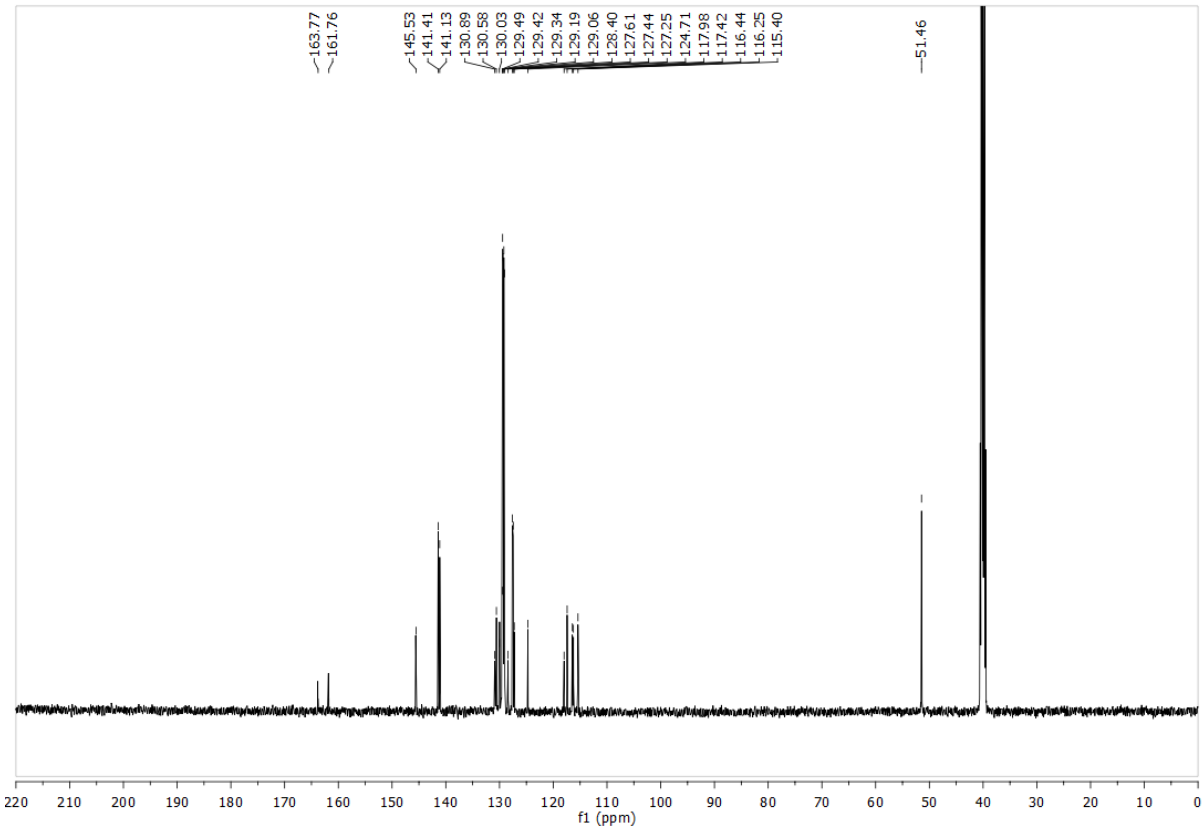
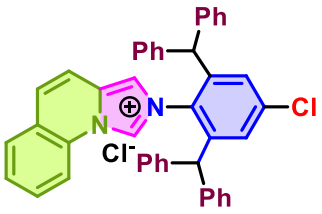
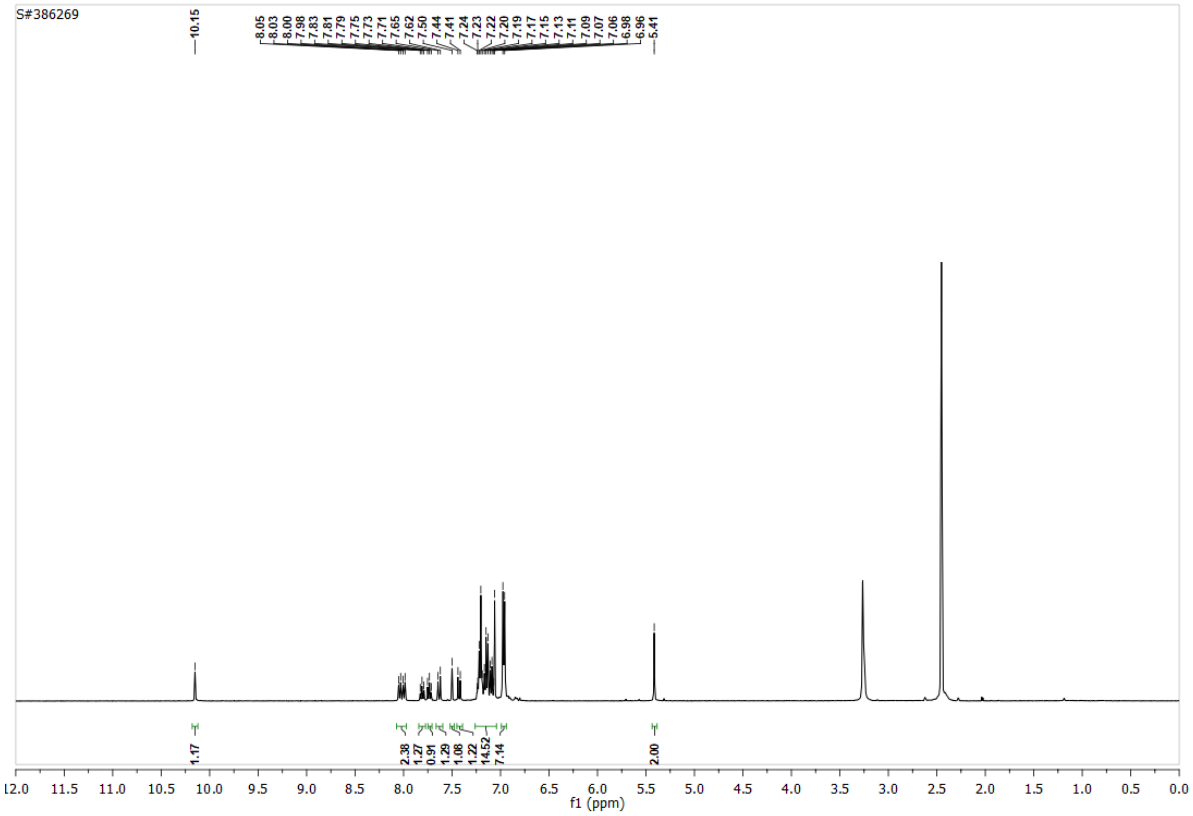


Figure S13. ^{1}H NMR and $^{13}C\{^{1}H\}$ NMR spectra of L4

L5



White solid. Yield: 87%. ^{1}H NMR (δ ppm, DMSO–d_6, 400 MHz): 10.13 (s, 1H), 8.01 (dd, J=15.1, 8.1 Hz, 2H), 7.81 (t, J=7.8 Hz, 1H), 7.73 (t, J=7.4 Hz, 1H), 7.50 (s, 1H), 7.43 (d, J=9.1 Hz, 1H), 7.25-7.05 (m, 12H), 6.97 (d, J=7.3 Hz, 8H), 6.93 (s, 2H), 5.41 (s, 2H), ^{13}C NMR (δ ppm DMSO–d_6, 100 MHz, proton decoupled): 144.75, 141.03, 136.21, 132.68, 130.58, 130.01, 129.32, 128.45, 127.49, 124.70, 117.88, 117.23, 113.56, 51.41. ESI-MS (ES+; $[M]^+$ m/z) calculated for $C_{43}H_{32}ClN_2^+$: 611.2249, observed 611.2248.



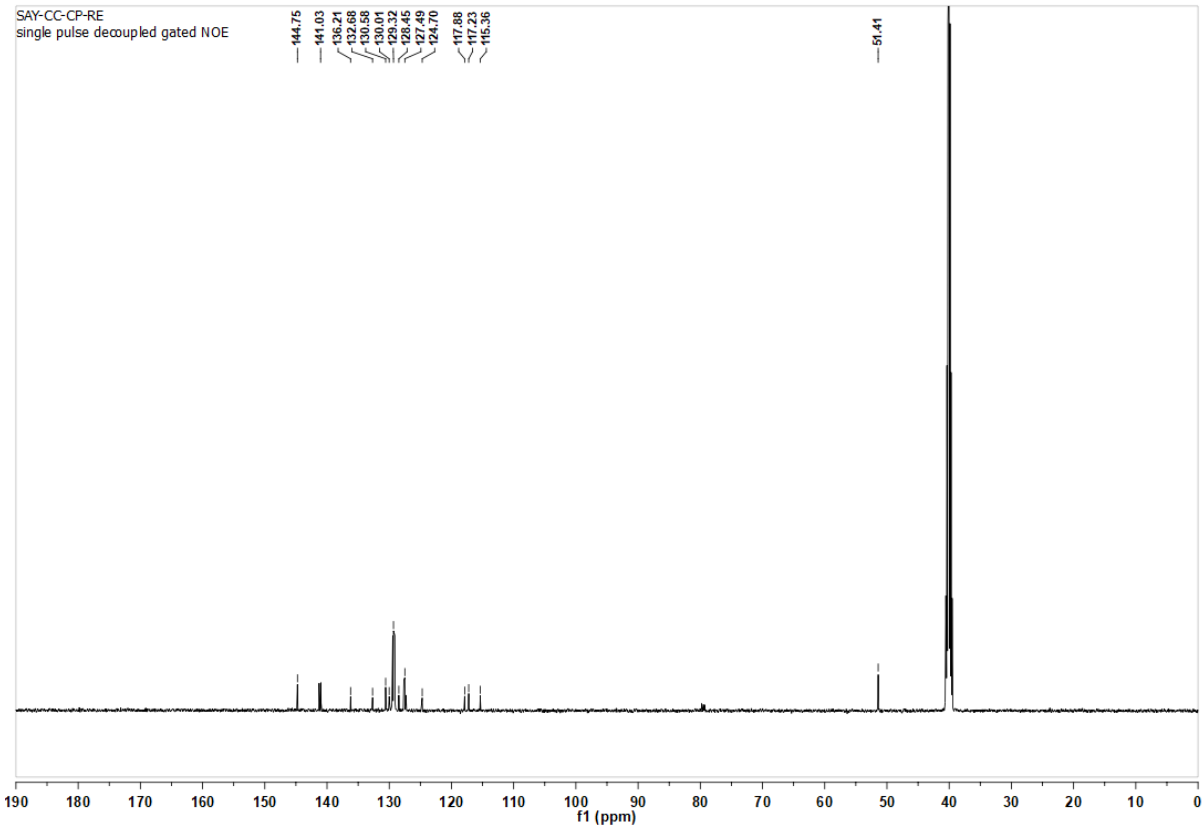
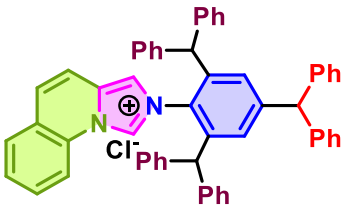
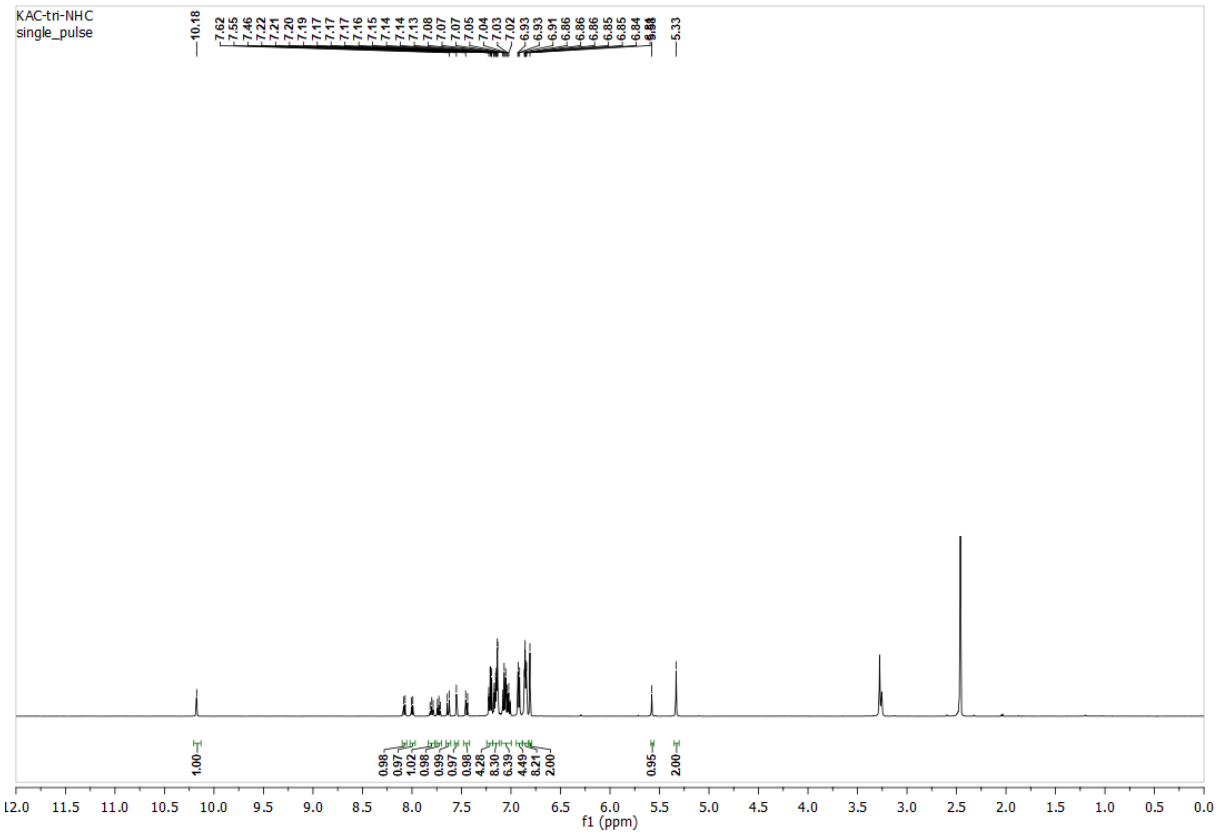


Figure S14. ^{1}H NMR and ^{13}C{^{1}H} NMR spectra of L5

L6



White solid. Yield: 81%. ^{1}H NMR (δ ppm, DMSO–d_6, 500 MHz): 10.18 (s, 1H), 8.08 (d, J=8.3, 1H), 8.00 (dd, J= 7.8, 1.2 Hz), 7.82-7.77 (m, 1H), 7.75-7.70 (m, 1H), 7.63 (d, J= 9.7 Hz, 1H), 7.55 (d, J=1.5 Hz, 1H), 7.45 (d, J= 9.7 Hz, 1H), 7.26-7.19 (m, 4H), 7.18-7.12 (m, 8H), 7.09-7.00 (m, 7H), 6.95-6.90 (m, 4H), 6.88-6.83 (m, 8H), 6.81 (s, 2H), 5.58(s, 1H), 5.33 (s, 2H), ^{13}C NMR (δ ppm DMSO–d_6, 100 MHz, proton decoupled): 146.70, 143.38, 141.98, 141.70, 131.83, 130.53, 130.38, 130.01, 129.42, 129.21, 128.91, 128.57, 127.23, 126.99, 124.75, 117.41, 115.50, 55.57, 51.31. ESI-MS (ES+; $[M]^+$ m/z) calculated for $C_{56}H_{43}N_2^+$:743.3240, observed: 743.3432.



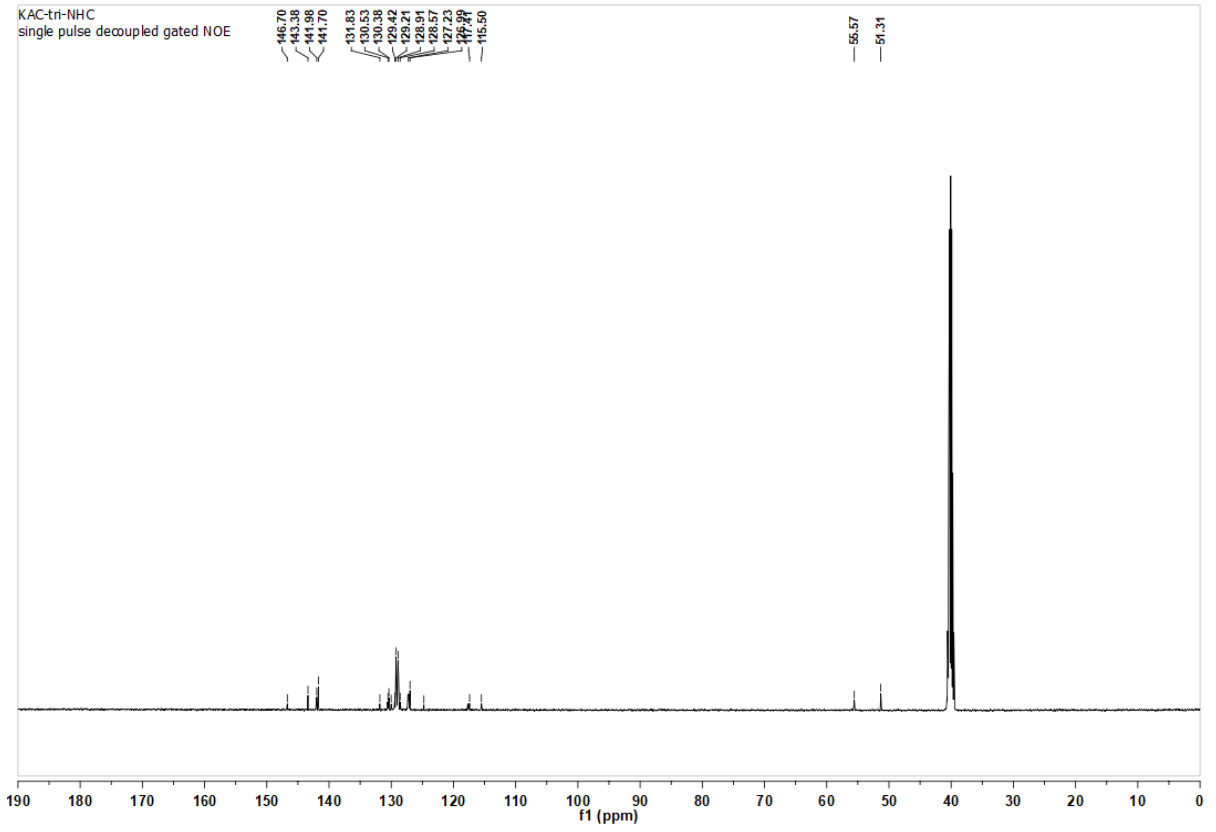
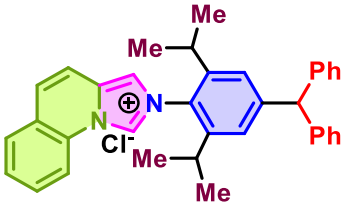
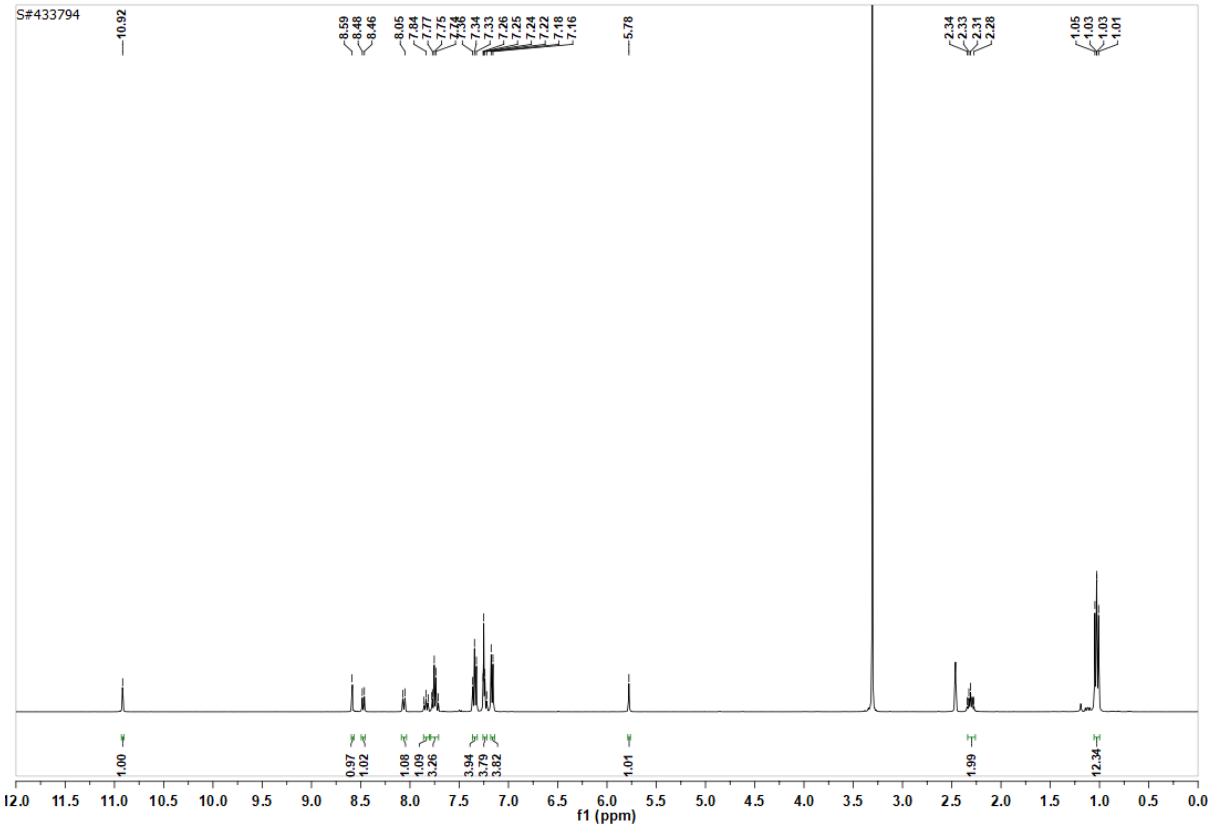


Figure S15. ^{1}H NMR and $^{13}C\{^{1}H\}$ NMR spectra of L7

L7



White solid. Yield: 81%. ^{1}H NMR (δ ppm, DMSO–d_6, 400 MHz): 10.92 (s, 1H), 8.59 (s, 1H), 8.47 (d, J = 8.3 Hz, 1H), 8.06 (d, J = 8.8 Hz, 1H), 7.84 (t, J = 8.4 Hz, 1H), 7.78 – 7.71 (m, 3H), 7.34 (t, J = 7.5 Hz, 4H), 7.27 – 7.22 (m, 4H), 7.17 (d, J = 7.3 Hz, 4H), 5.78 (s, 1H), 2.34 – 2.22 (m, 2H), 1.03 (dd, J = 8.0, 7.1 Hz, 12H). ^{13}C NMR (δ ppm DMSO–d_6, 100 MHz, proton decoupled):147.93,145.68, 143.73, 130.87,130.12,129.94,129.45,129.07,127.62,127.12,125.55,125.05,118.27,117.73,115.89, 56.26, 28.26, 24.52. ESI-MS (ES+; $[M]^+$ m/z) calculated for $C_{36}H_{33}N_2^+$:495.2794, observed:495.2817.



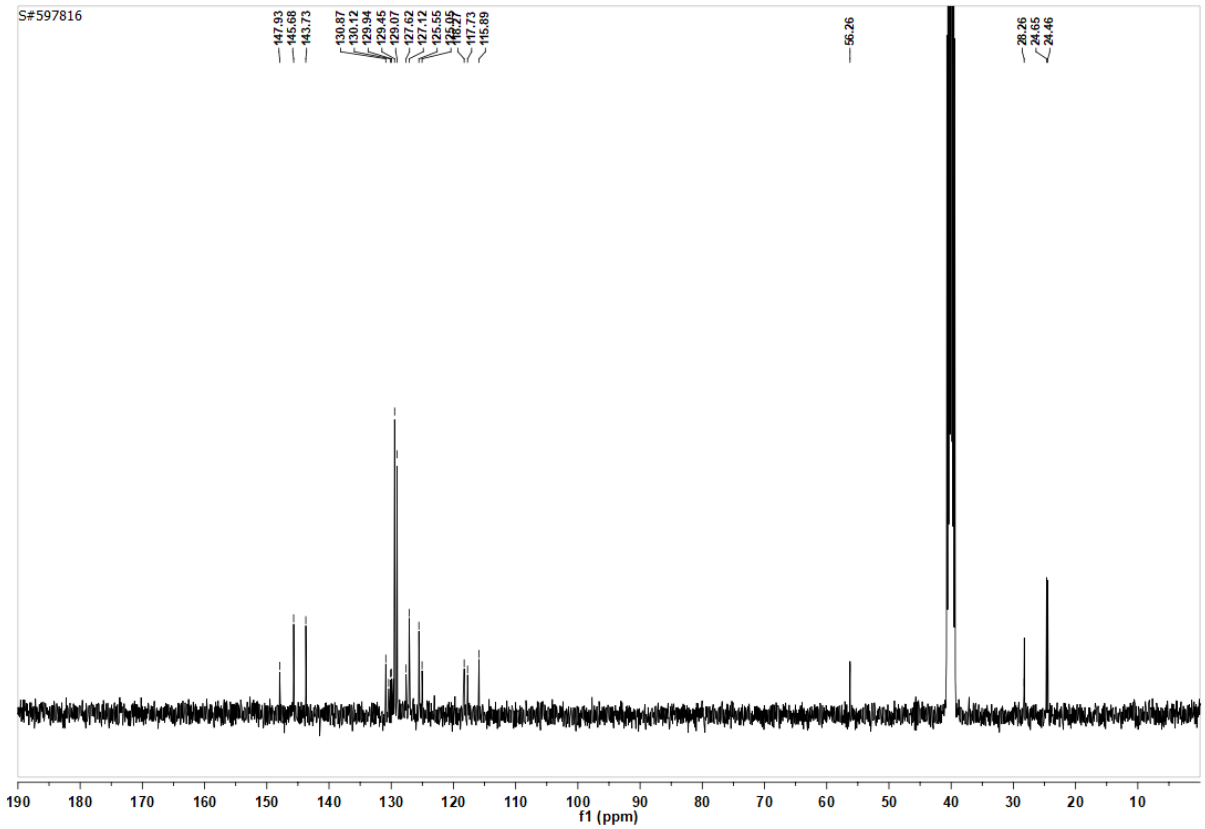
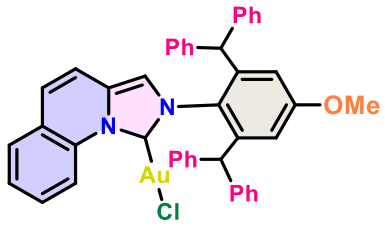
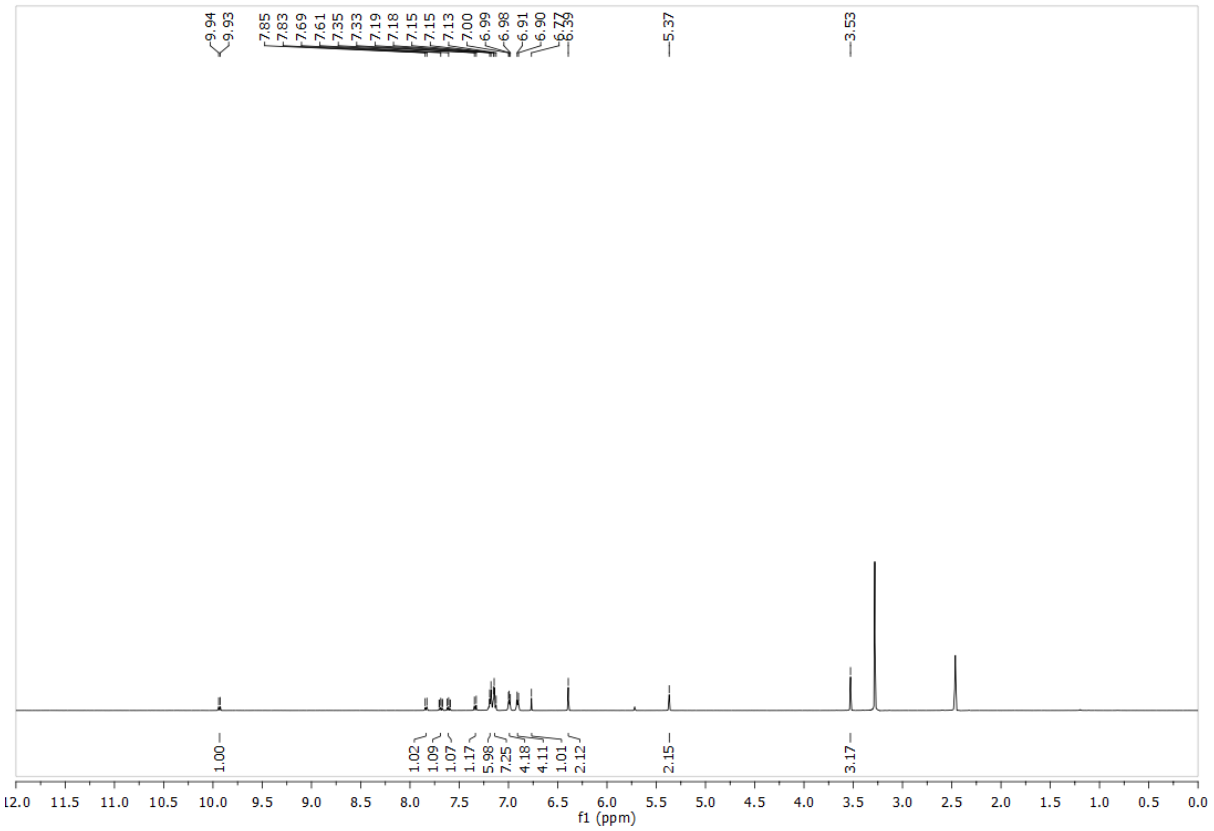
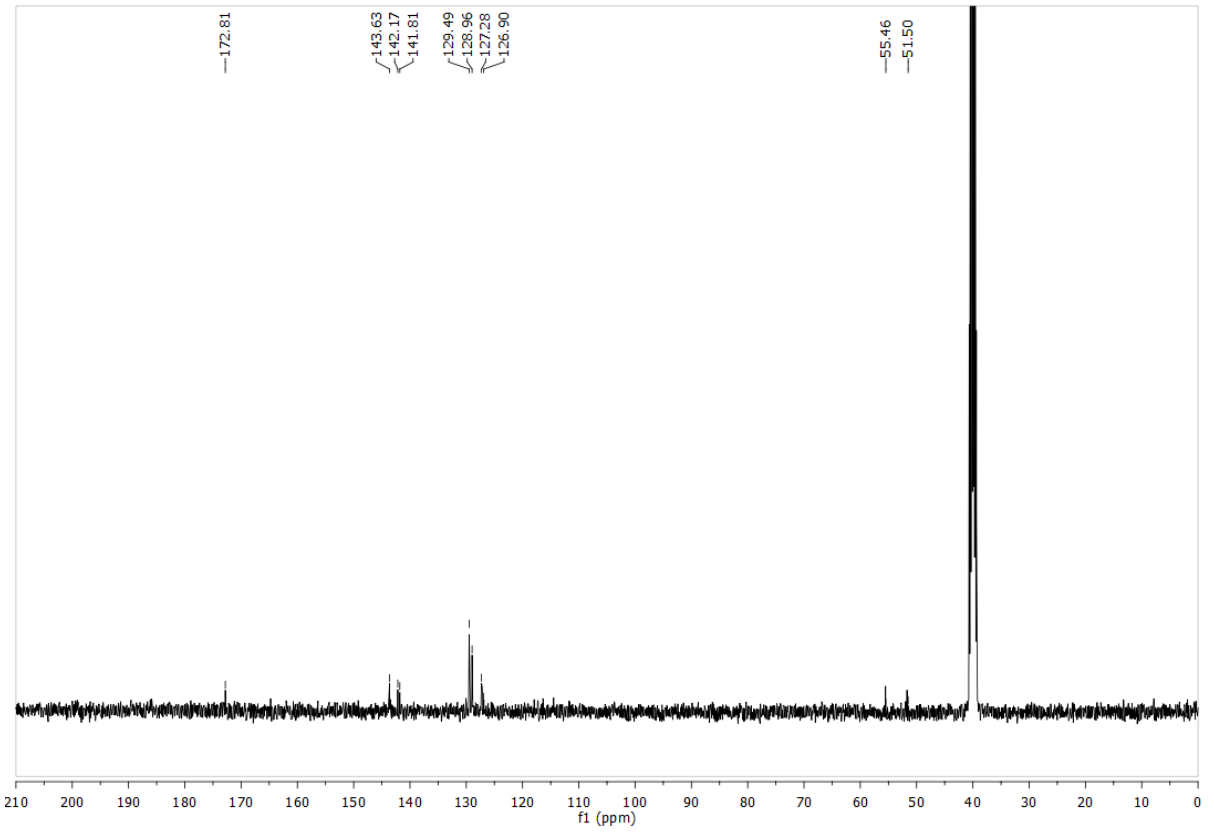


Figure S16. ^{1}H NMR and $^{13}C\{^{1}H\}$ NMR spectra of L7

Au-L1




9.94
9.93
7.85
7.83
7.69
7.61
7.35
7.33
7.19
7.18
7.15
7.15
7.13
7.00
6.99
6.98
6.91
6.90
6.77
6.76
5.37
3.53
1.00
1.02
1.09
1.07
1.17
5.98
7.25
4.18
4.11
1.01
2.12
2.15
3.17
f1 (ppm)


172.81
143.63
142.17
141.81
129.49
128.96
127.28
126.90
55.46
51.50
f1 (ppm)

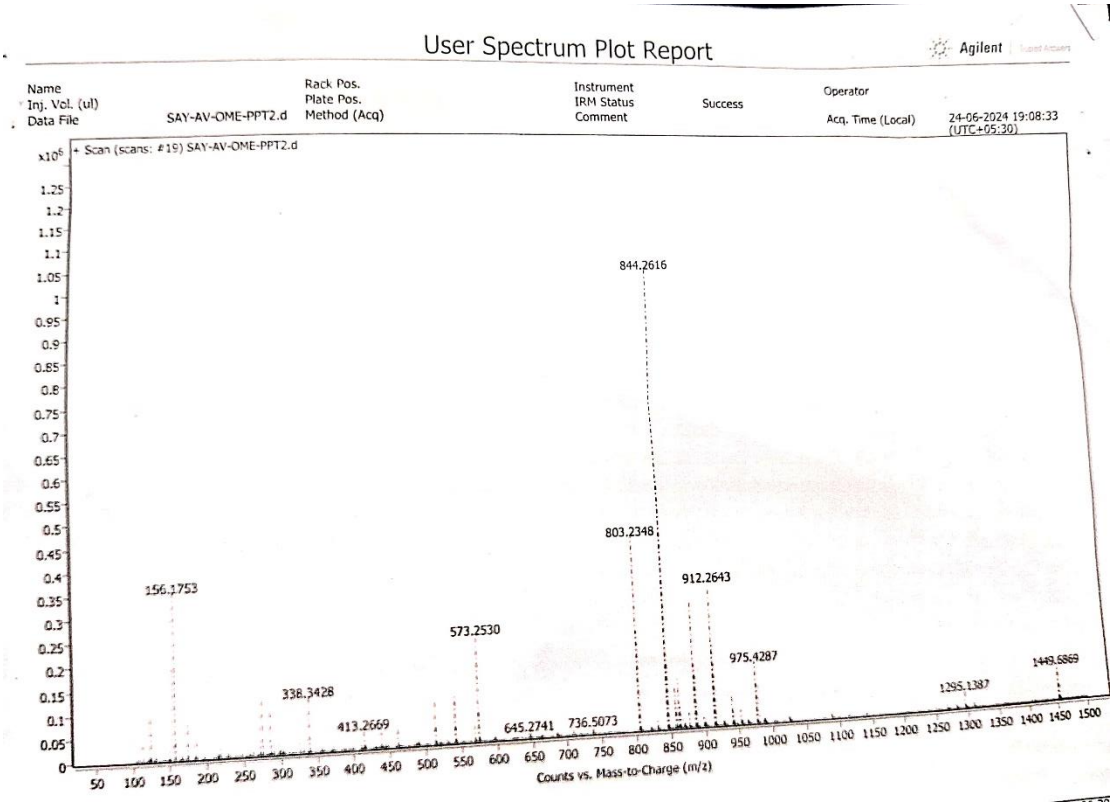
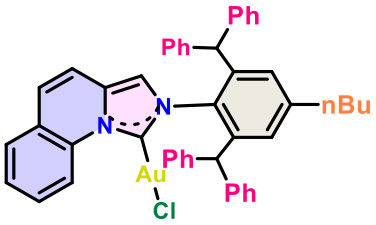
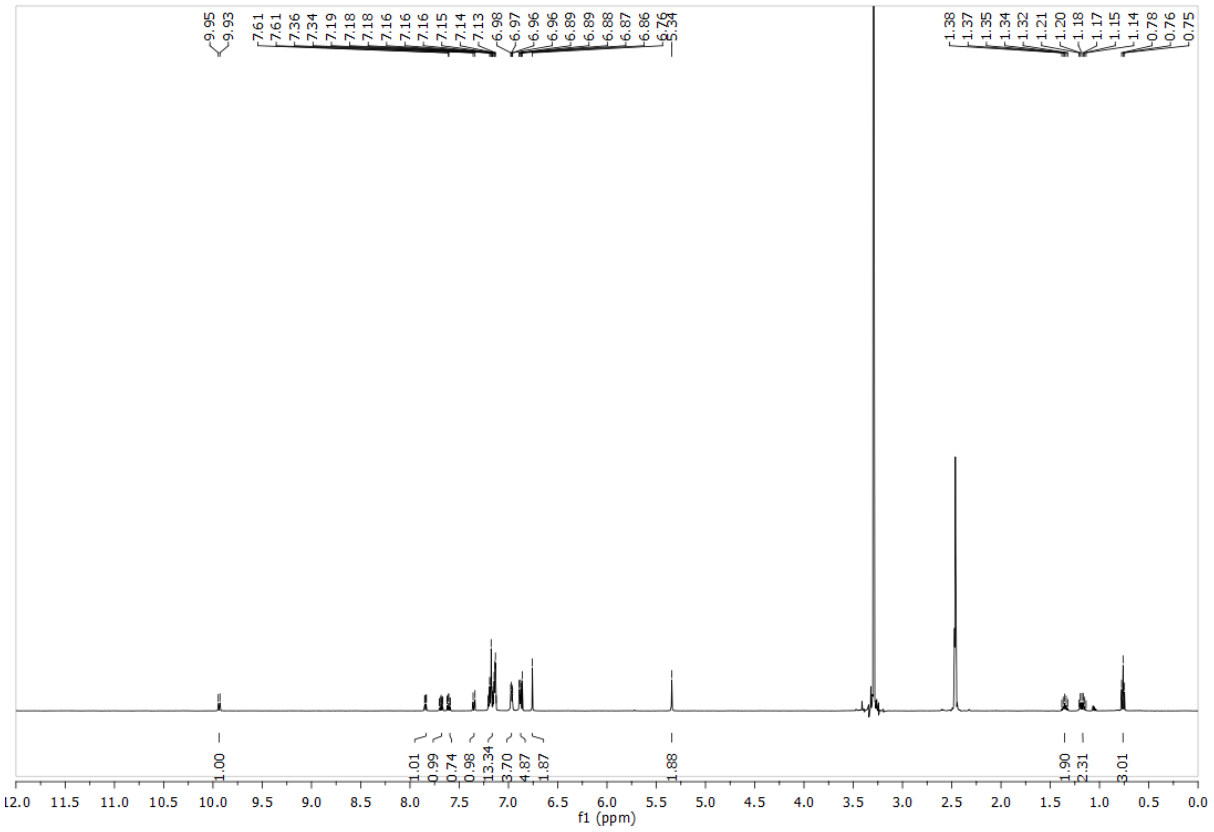


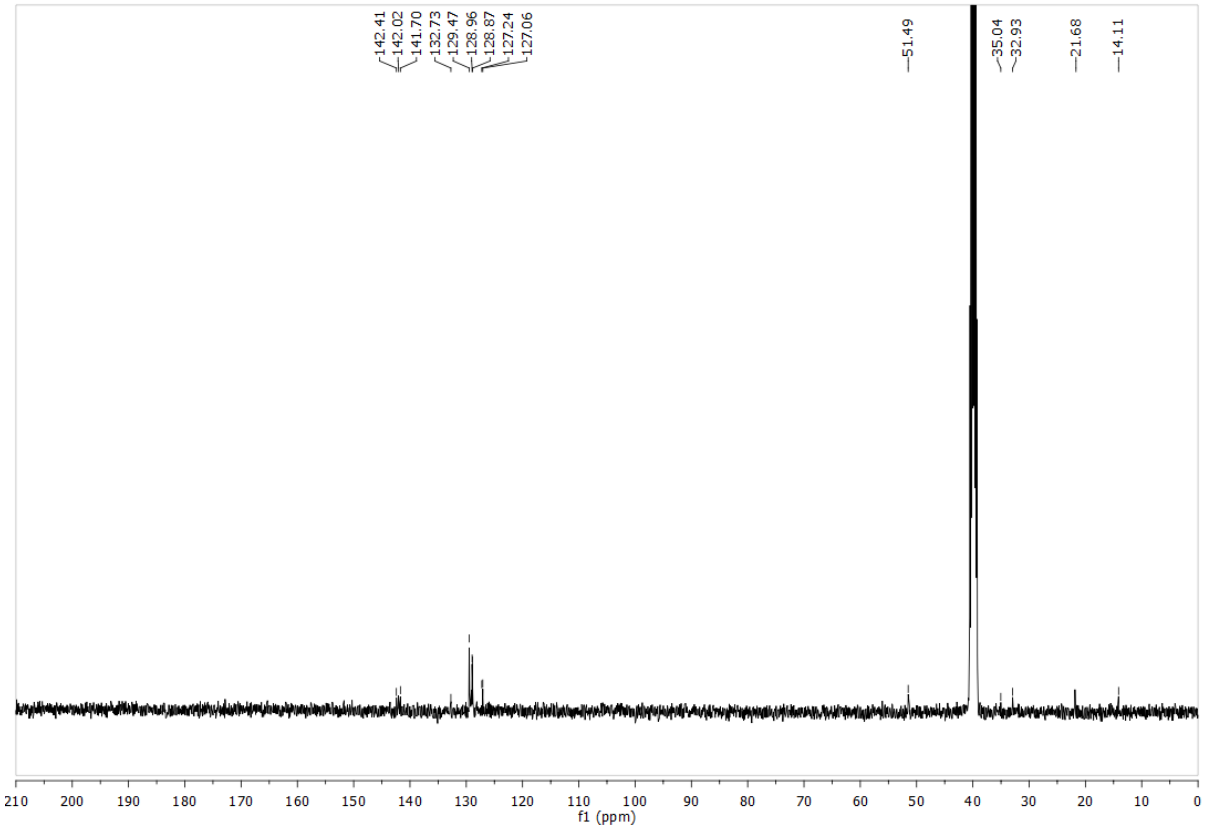
Figure S17. ^{1}H NMR and $^{13}C\{^{1}H\}$ NMR, ESI-MS spectra of Au-L1.

Au-L2



.


9.95
9.93
7.61
7.61
7.36
7.34
7.19
7.18
7.18
7.16
7.16
7.16
7.15
7.14
7.13
6.98
6.97
6.96
6.96
6.89
6.89
6.88
6.87
6.86
6.76
5.34
1.38
1.37
1.35
1.34
1.32
1.21
1.20
1.18
1.17
1.15
1.14
0.78
0.76
0.75
1.00
1.01
0.99
0.74
0.98
3.34
3.70
4.87
1.87
1.88
1.90
2.31
3.01
f1 (ppm)


142.41
142.02
141.70
132.73
129.47
128.96
128.87
127.24
127.06
51.49
35.04
32.93
21.68
14.11
f1 (ppm)

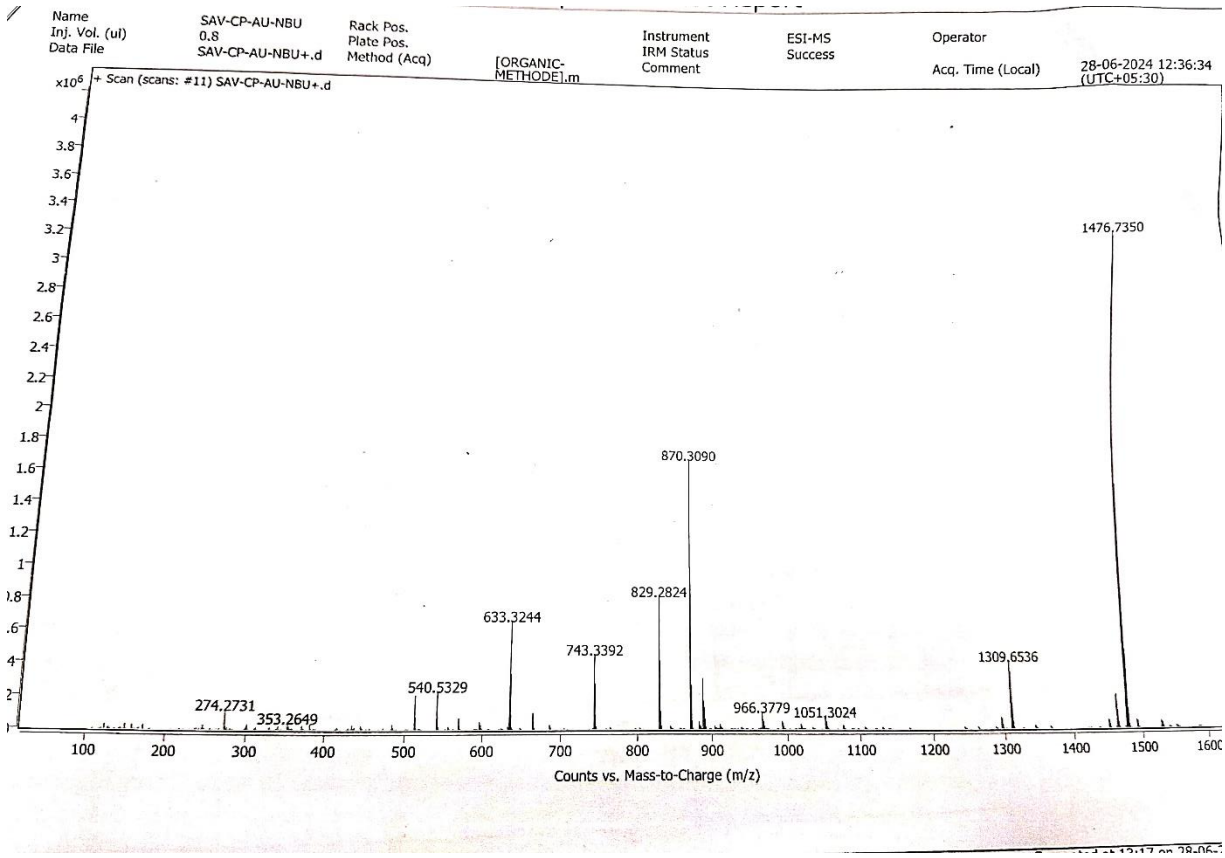
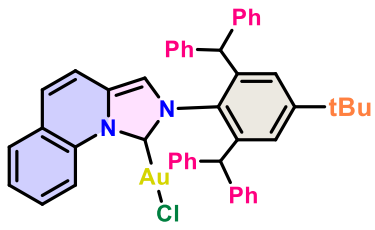
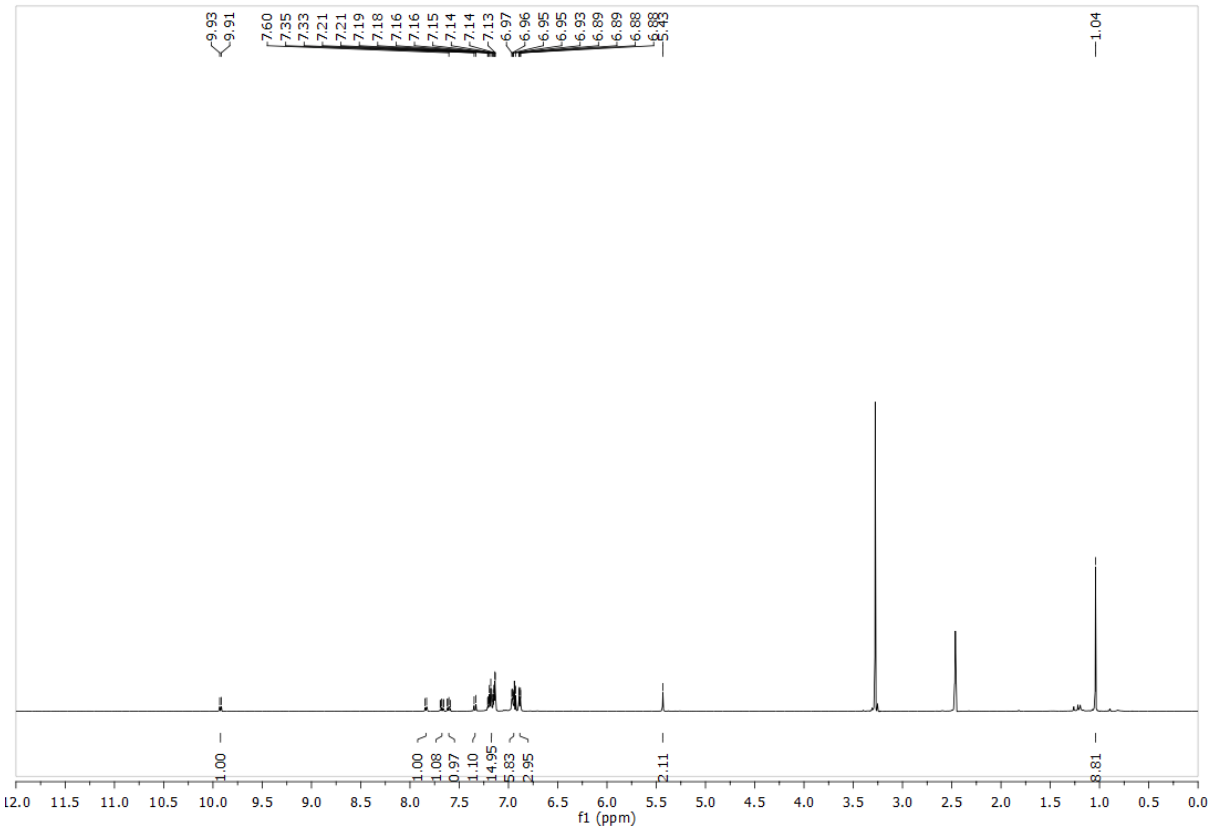
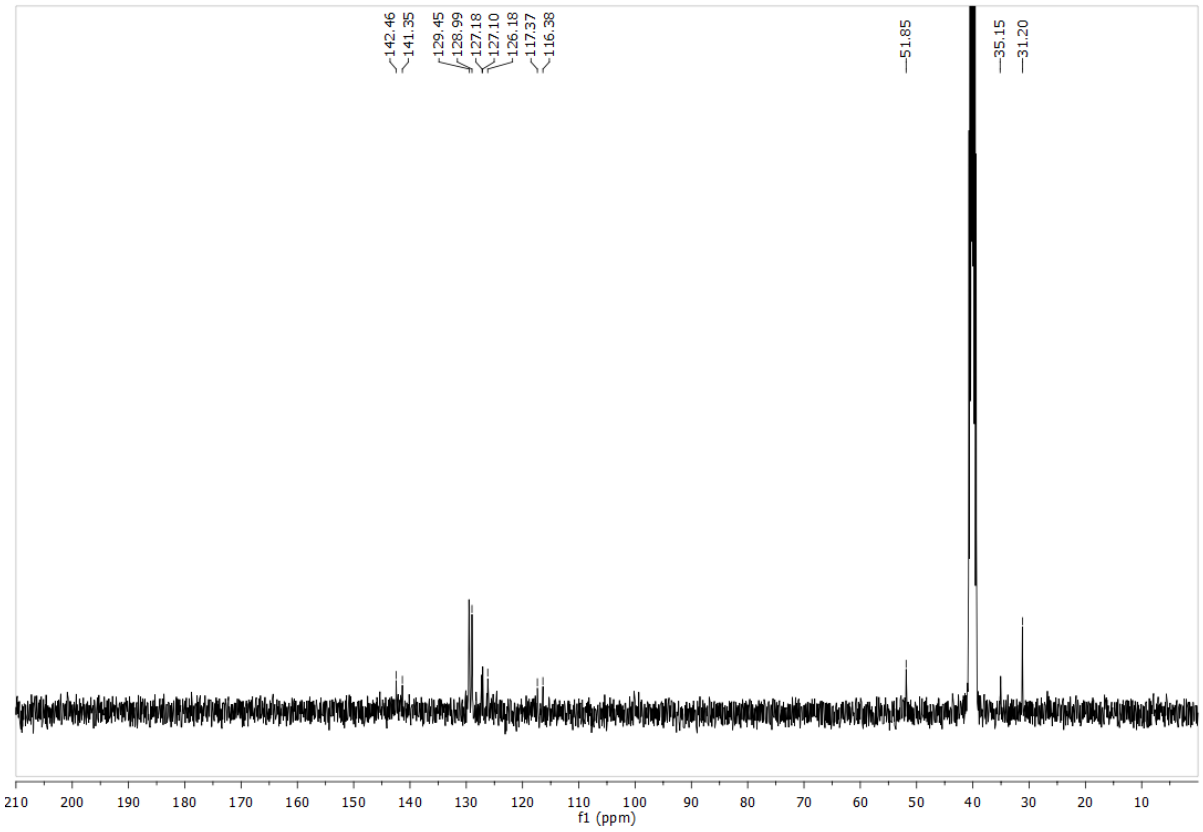


Figure S18. ^{1}H NMR and $^{13}C\{^{1}H\}$ NMR, ESI-MS spectra of AuL2

Au-L3




9.93
9.91
7.60
7.35
7.33
7.21
7.21
7.19
7.18
7.16
7.16
7.15
7.14
7.14
7.13
6.97
6.96
6.95
6.95
6.93
6.89
6.89
6.88
6.88
5.43
1.04
1.00
1.00
1.08
0.97
1.10
4.95
5.83
2.95
2.11
8.81
12.0
11.5
11.0
10.5
10.0
9.5
9.0
8.5
8.0
7.5
7.0
6.5
6.0
5.5
5.0
4.5
4.0
3.5
3.0
2.5
2.0
1.5
1.0
0.5
0.0
f1 (ppm)



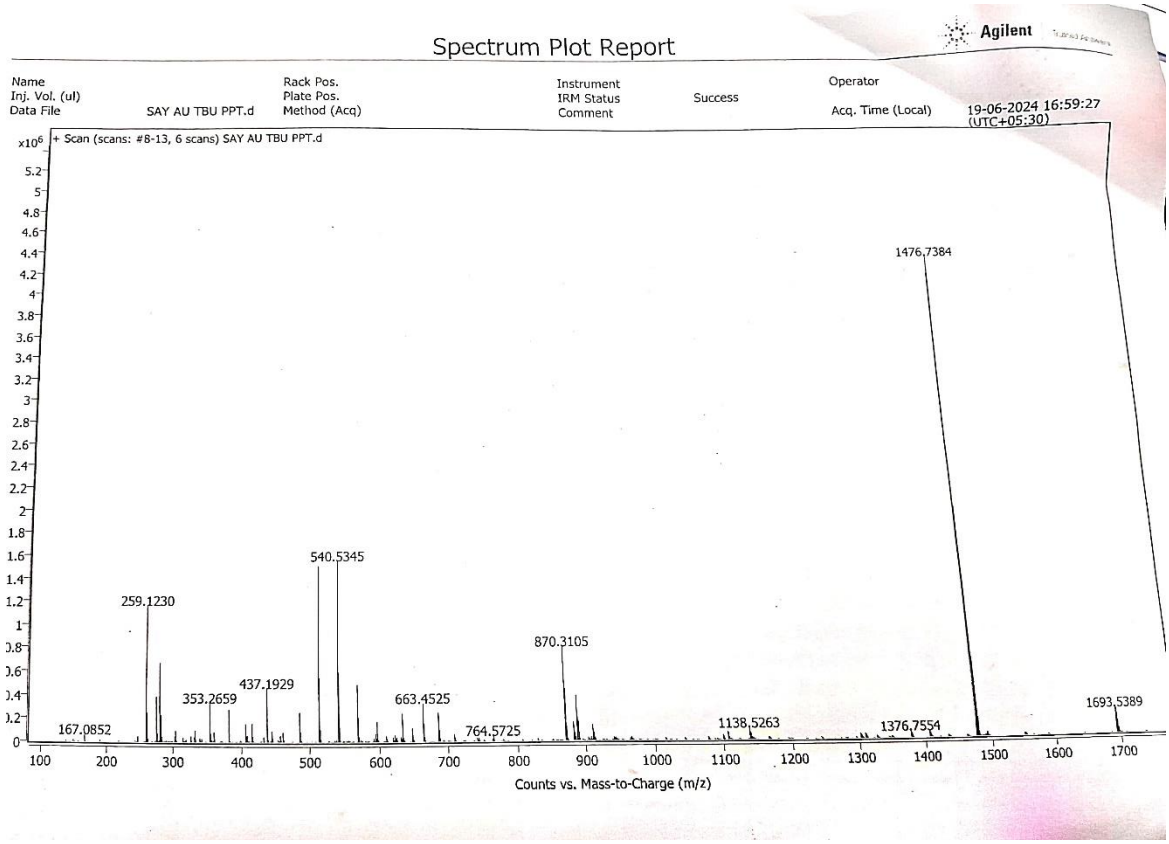
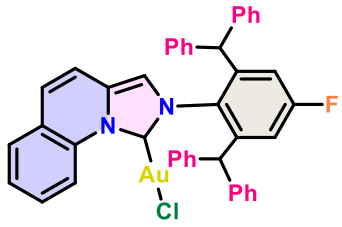
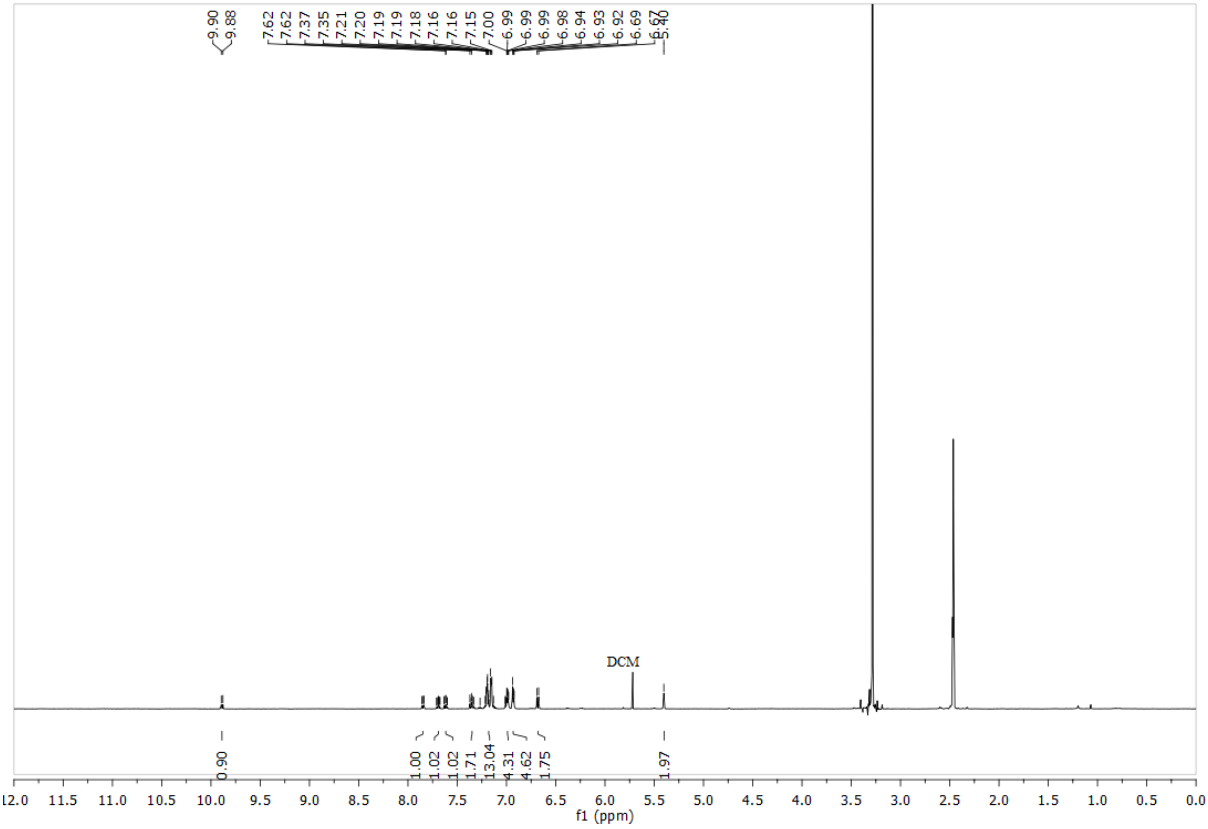
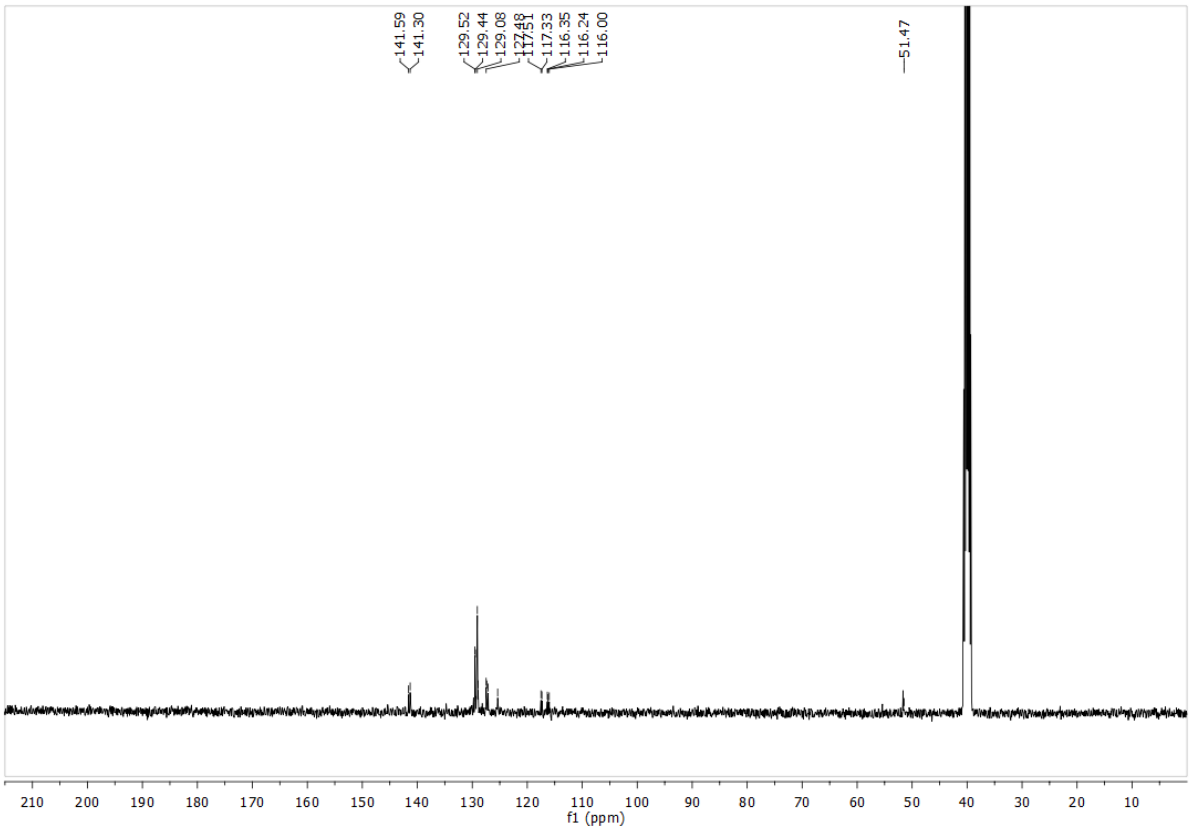


Figure S19. ^{1}H NMR and $^{13}C\{^{1}H\}$ NMR, ESI-MS spectra of AuL3.

Au-L4


Ph
Ph
N
N
F
Ph
Au
Cl
Ph


9.90
9.88
7.62
7.62
7.37
7.35
7.21
7.20
7.19
7.19
7.18
7.16
7.16
7.15
7.00
6.99
6.99
6.99
6.98
6.94
6.93
6.92
6.69
6.67
6.60
DCM
0.90
1.00
1.02
1.02
1.71
13.04
4.31
4.62
1.75
1.97
12.0
11.5
11.0
10.5
10.0
9.5
9.0
8.5
8.0
7.5
7.0
6.5
6.0
5.5
5.0
4.5
4.0
3.5
3.0
2.5
2.0
1.5
1.0
0.5
0.0
f1 (ppm)



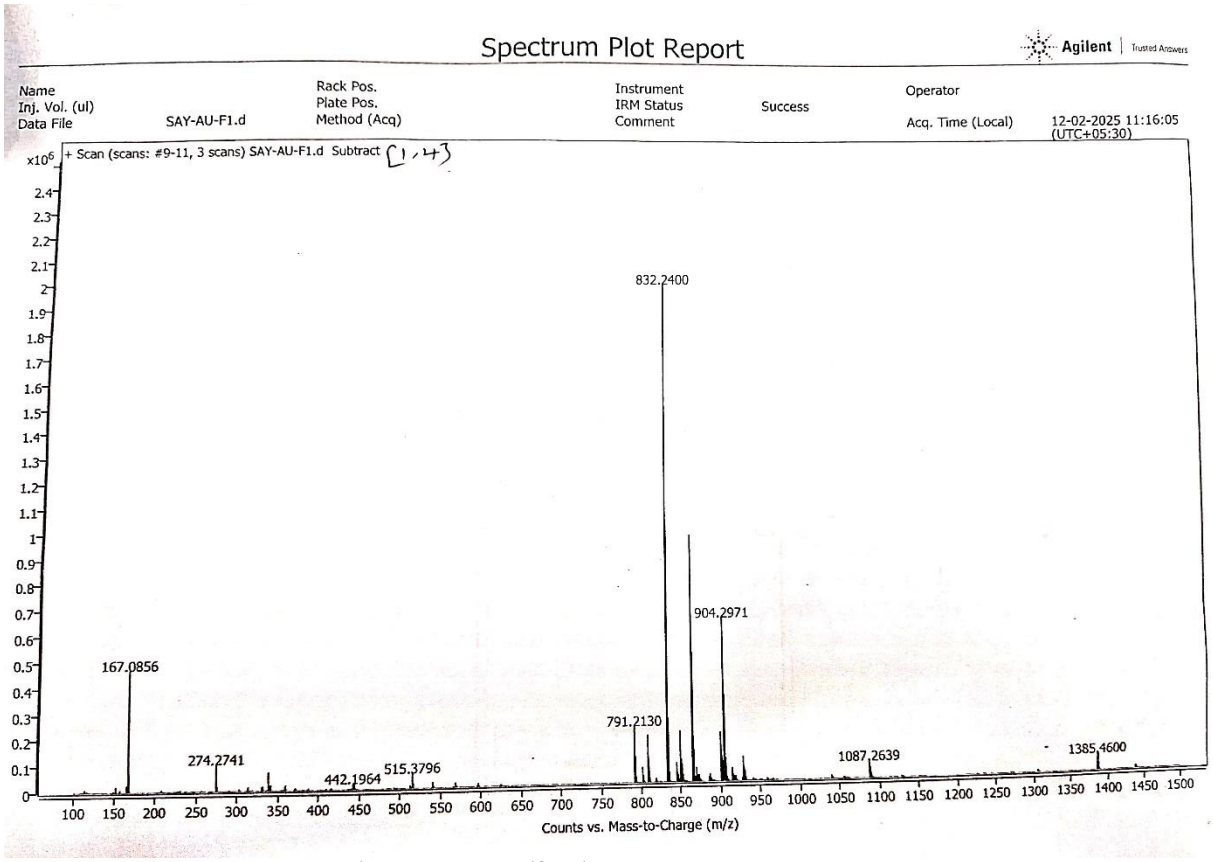
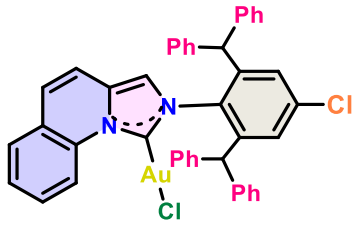
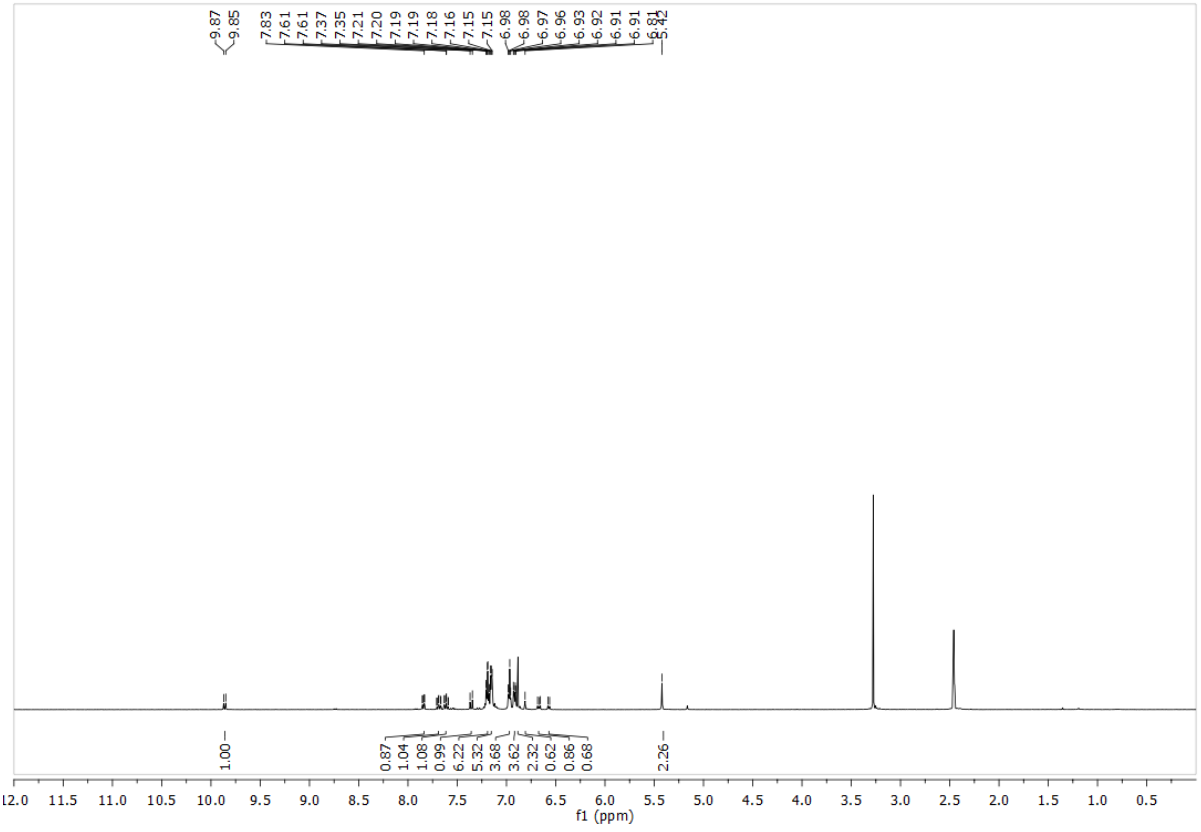
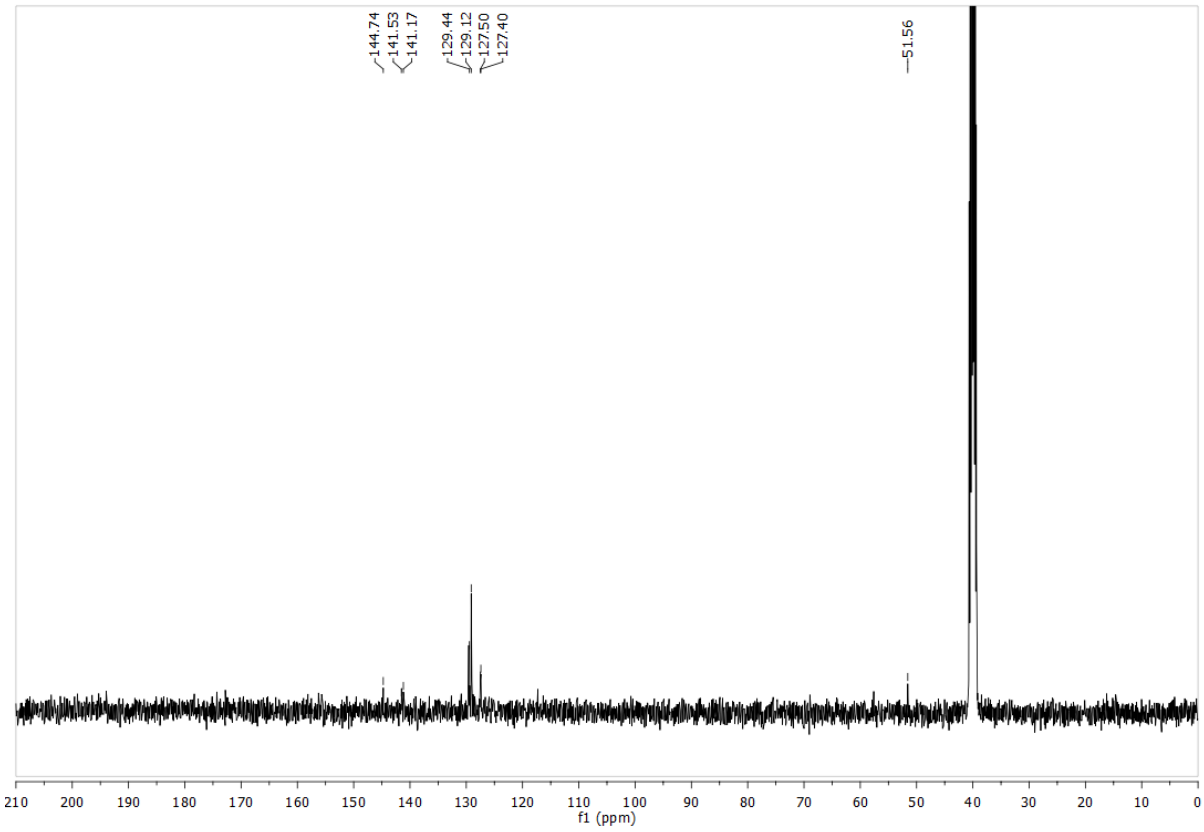


Figure S20. ^{1}H NMR and $^{13}C\{^{1}H\}$ NMR, ESI-MS spectra of AuL4

Au-L5


Ph
Ph
N
N
Cl
Ph
Au
Cl
Ph


9.87
9.85
7.83
7.61
7.61
7.37
7.35
7.21
7.20
7.19
7.19
7.18
7.16
7.15
7.15
6.98
6.98
6.97
6.96
6.93
6.92
6.91
6.91
6.81
6.42
1.00
0.87
1.04
1.08
0.99
6.22
5.32
3.68
3.62
2.32
0.62
0.86
0.68
2.26
12.0
11.5
11.0
10.5
10.0
9.5
9.0
8.5
8.0
7.5
7.0
6.5
6.0
5.5
5.0
4.5
4.0
3.5
3.0
2.5
2.0
1.5
1.0
0.5
f1 (ppm)



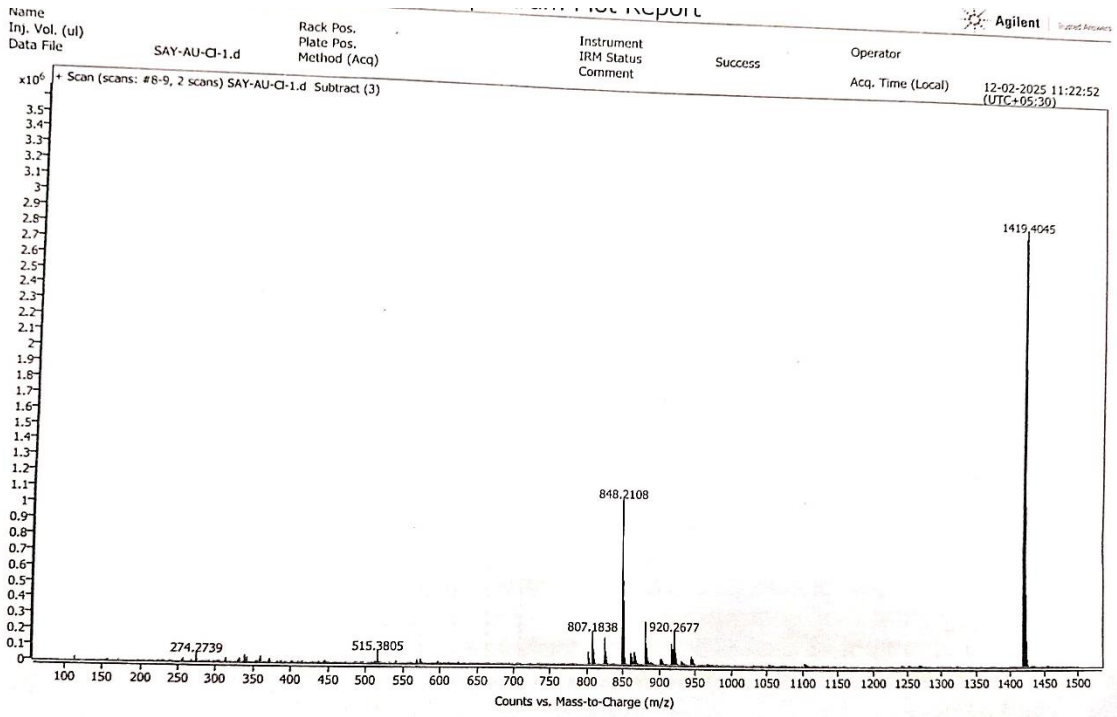
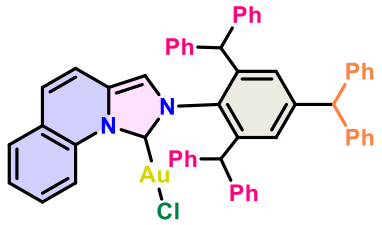
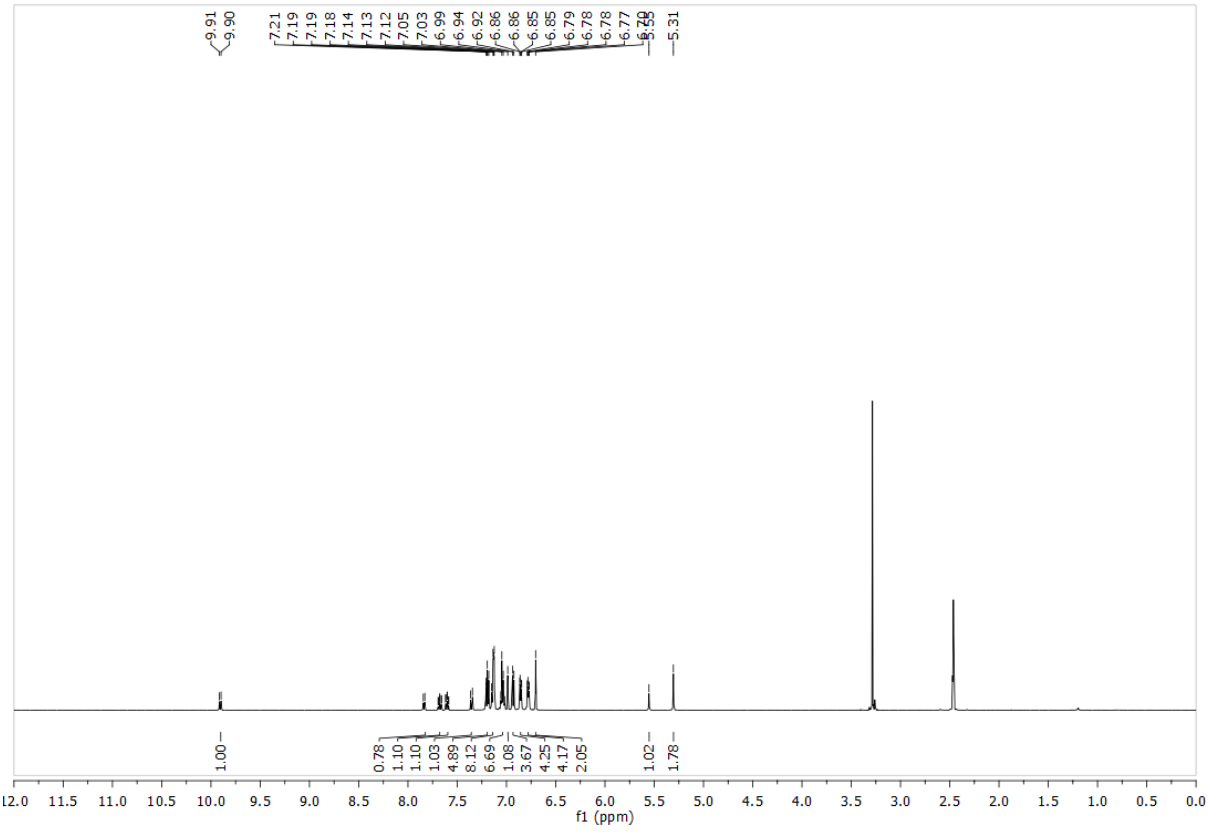
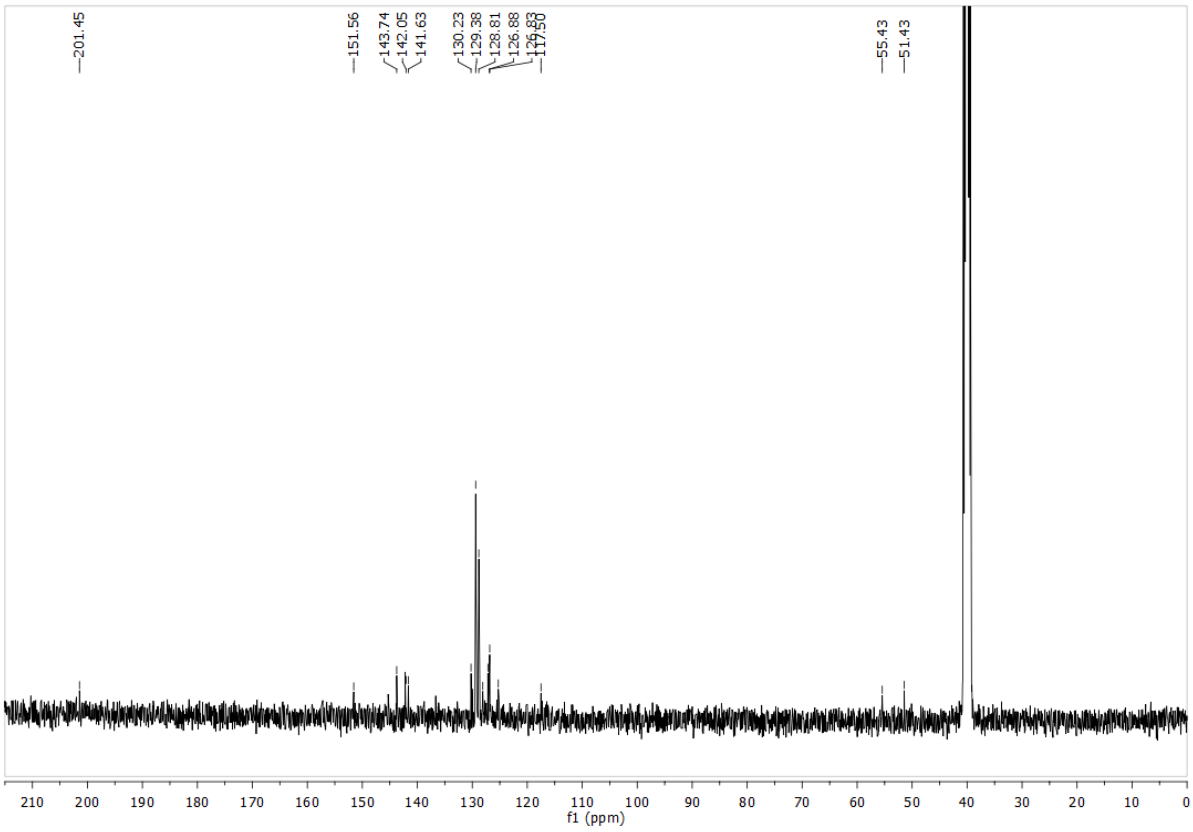


Figure S21. ^{1}H NMR and $^{13}C\{^{1}H\}$ NMR, ESI-MS spectra of AuL5

Au-L6


Ph
Ph
Ph
N
N
Ph
Au
Ph
Cl


9.91
9.90
7.21
7.19
7.19
7.18
7.14
7.13
7.12
7.05
7.03
6.99
6.94
6.92
6.86
6.86
6.85
6.85
6.79
6.78
6.78
6.77
6.59
5.55
5.31
1.00
0.78
1.10
1.10
1.03
4.89
8.12
6.69
1.08
3.67
4.25
4.17
2.05
1.02
1.78
12.0
11.5
11.0
10.5
10.0
9.5
9.0
8.5
8.0
7.5
7.0
6.5
6.0
5.5
5.0
4.5
4.0
3.5
3.0
2.5
2.0
1.5
1.0
0.5
0.0
f1 (ppm)



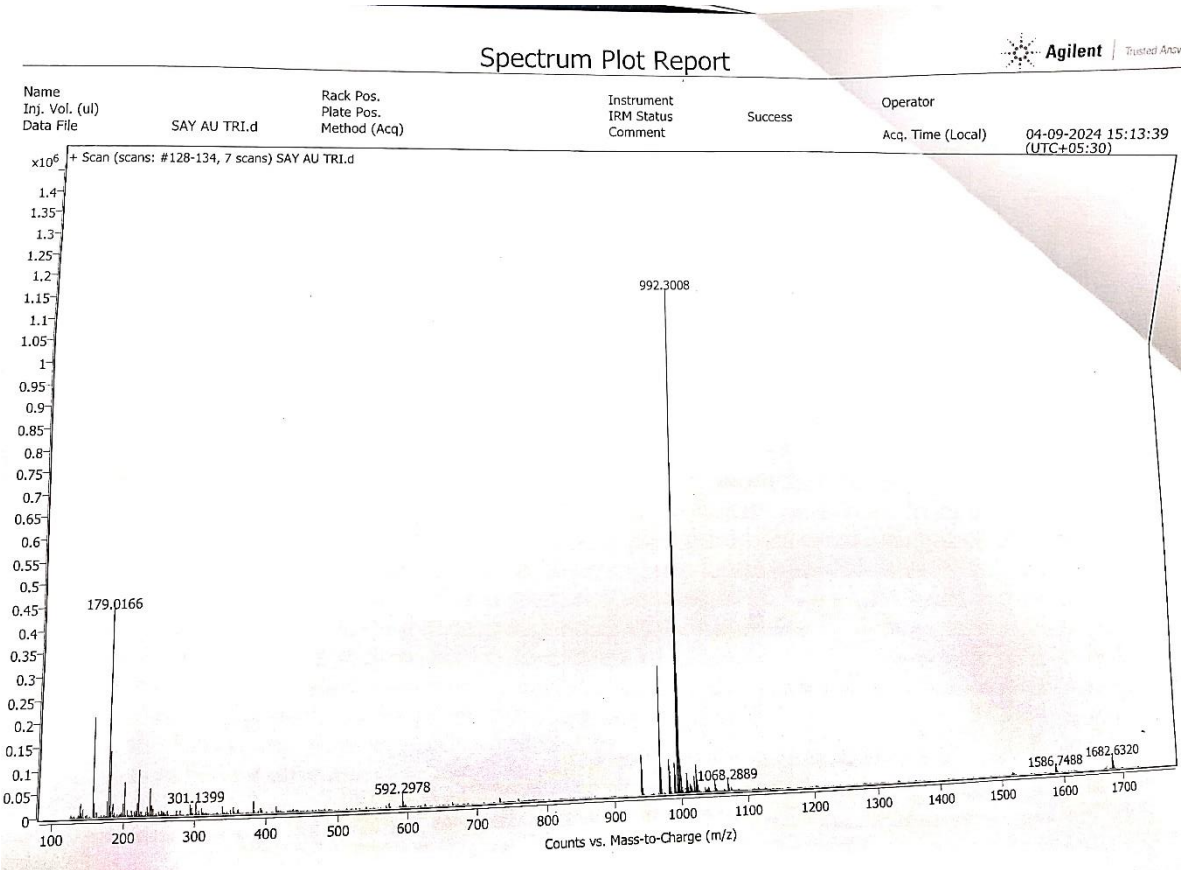
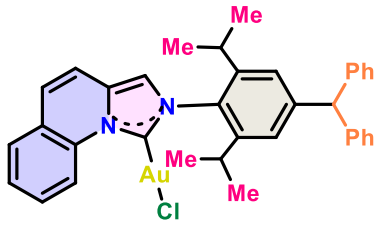
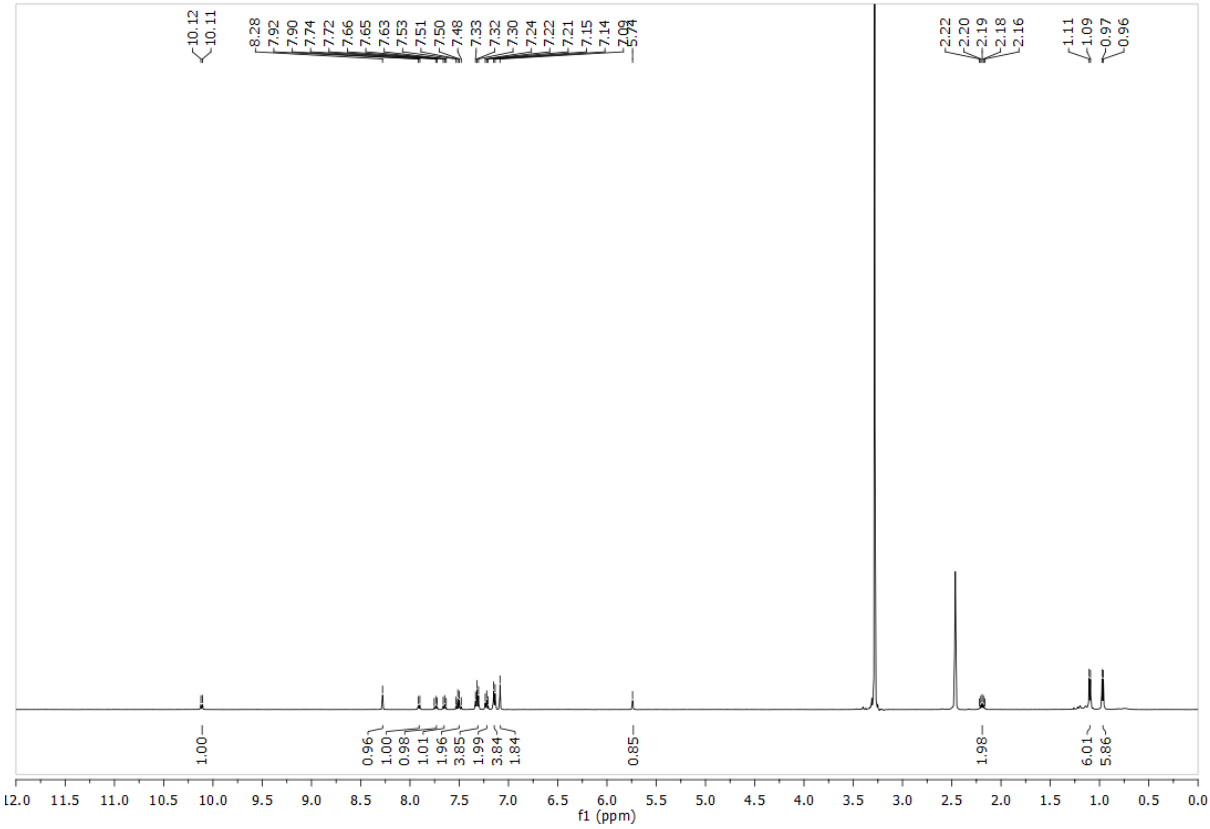


Figure S22. ^{1}H NMR and ^{13}C{^{1}H} NMR, ESI-MS spectra of AuL6.

Au-L7


Me
Me
Ph
Ph
N
N
Me
Me
Au
Cl


10.12
10.11
8.28
7.92
7.90
7.74
7.72
7.66
7.65
7.63
7.53
7.51
7.50
7.48
7.33
7.32
7.30
7.24
7.22
7.21
7.15
7.14
7.09
5.74
2.22
2.20
2.19
2.18
2.16
1.11
1.09
0.97
0.96
1.00
0.96
1.00
0.98
1.01
1.96
3.85
1.99
3.84
1.84
0.85
1.98
6.01
5.86
12.0
11.5
11.0
10.5
10.0
9.5
9.0
8.5
8.0
7.5
7.0
6.5
6.0
5.5
5.0
4.5
4.0
3.5
3.0
2.5
2.0
1.5
1.0
0.5
0.0
f1 (ppm)

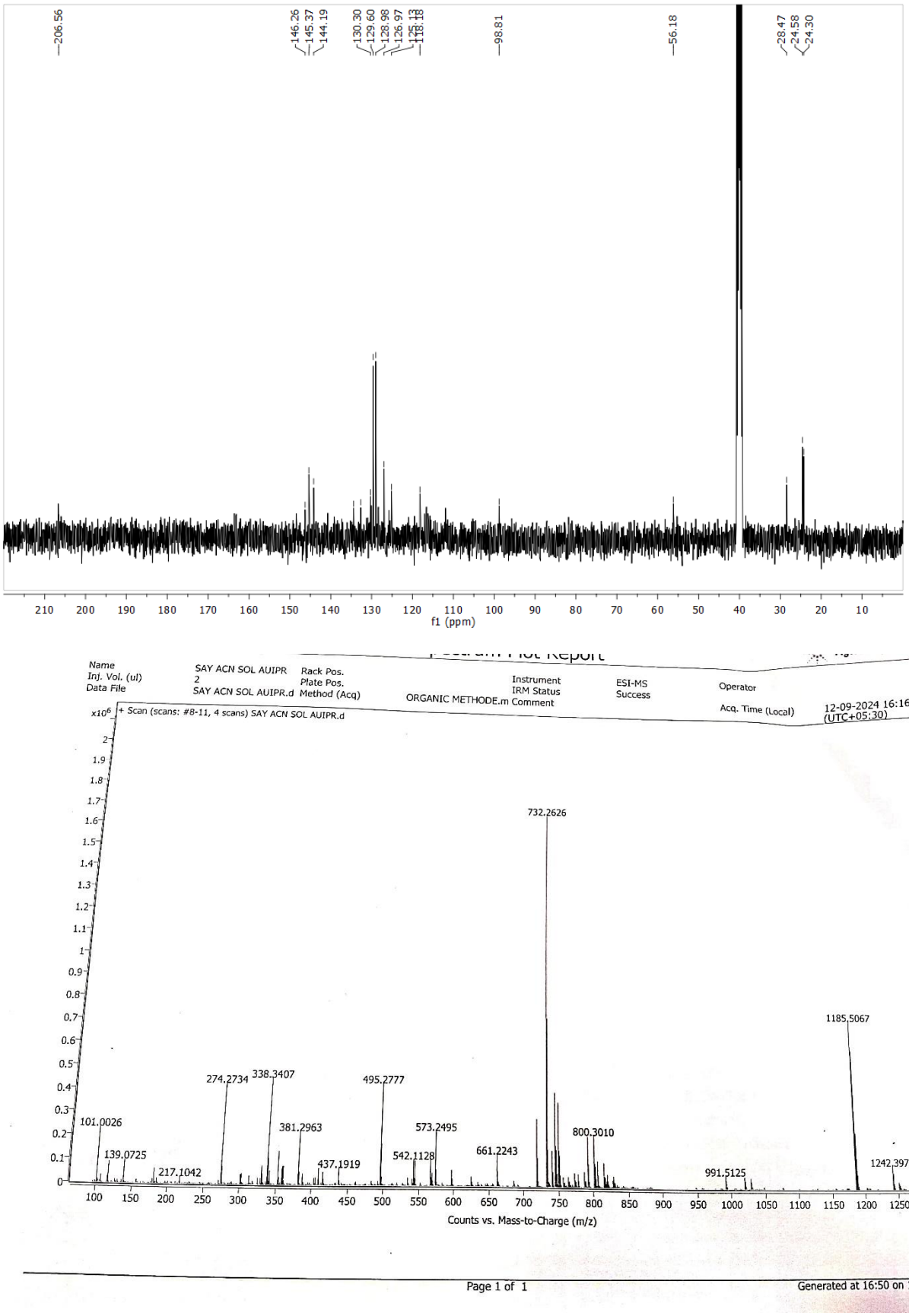


Figure S23. ^{1}H NMR and ^{13}C{^{1}H} NMR, ESI-MS spectra of AuL7.

Table S1: Structure description of gold complexes

	AuL2	**AuL3**	**AuL5**	**AuL7**
CCDC	2432305	2432303	2432304	2433312
Chemical formula	$C_{47}H_{40}AuClN_2$	$C_{47}H_{40}AuClN_2$	$C_{43}H_{31}AuCl_2N_2$	$C_{37}H_{34}AuCl_4N_2$
Formula weight	865.22	865.22	843.610	845.43
Temperature	100(2)	100(2)	100(2)	100(2)
Wavelength	0.71073	0.71073	0.71073	0.71073
Crystal size	0.14 × 0.12 × 0.1	0.14 × 0.12 × 0.1	0.14 × 0.12 × 0.1	0.12 × 0.11 × 0.1
Crystal system	Orthorhombic	Orthorhombic	Monoclinic	Monoclinic
Space group	Pbca	Pbca	C2/c	$P2_1/n$
Unit cell dimensions				
a (Å)	90	90	90	90
β (Å)	90	90	92.274(5)	103.8670(10)
γ (Å)	90	90	90	90
a	18.2277(5)	18.8209(5)	20.900(3)	13.8388(4)
b	19.7090(5)	18.3643(5)	19.148(4)	15.3932(4)
c	20.7662(6)	21.8306(5)	18.831(3)	16.2823(5)
Volume	7460.3(4)	7545.4(3)	7530(2)	3367.42(17)
Z	8	8	8	4
Density (calculated)	1.541	1.523	1.488	1.668
Absorption coefficient	4.052	4.006	4.081	4.716
F(000)	3456.0	3456.0	3321.0	8389
Goodness-of-fit on F^2	1.042	1.081	1.024	1.049
Final R indices I>2σ(I)	R_1=0.0250, wR_2=0.0480	R_1=0.0245, wR_2=0.0460	R_1=0.0286, wR_2=0.0608	R_1=0.0745, wR_2=0.0713

R indices (all data)	R_1=0.0387, wR_2=0.0517	R_1=0.0424, wR_2=0.0542	R_1=0.0382, wR_2=0.0647	R_1=0.0346, wR_2=0.0274

Table S2: Selected bond distances (Å) and bond angles (°) for gold complexes.

Bond distance(Å)	**AuL2**	**AuL3**	**AuL5**	**AuL7**
C1-N1	1.355(3)	1.357(3)	1.359(3)	1.349(4)
C1-N2	1.367(3)	1.364(4)	1.356(4)	1.370(4)
C12-N1	1.445(3)	1.450(3)	1.441(3)	1.449(4)
Au1-C1	1.978(2)	1.983(3)	1.987(3)	1.967(4)
Au1-Cl1	2.2671(6)	2.2625(7)	2.2689(9)	2.289(15)
Bond angle (°)				
Cl1-Au1-C1	173.94(7)	174.48(8)	174.40(8)	176.1(4)
Au1-C1-N1	119.61(17)	122.2(2)	124.1(2)	121.6(2)
Au1-C1-N2	136.02(19)	132.9(2)	130.2(2)	133.8(2)
N1-C1-N2	104.3(2)	104.6(2)	104.6(2)	104.4(3)
C1-N1-C12	122.7(2)	123.0(2)	124.6(2)	124.7(3)

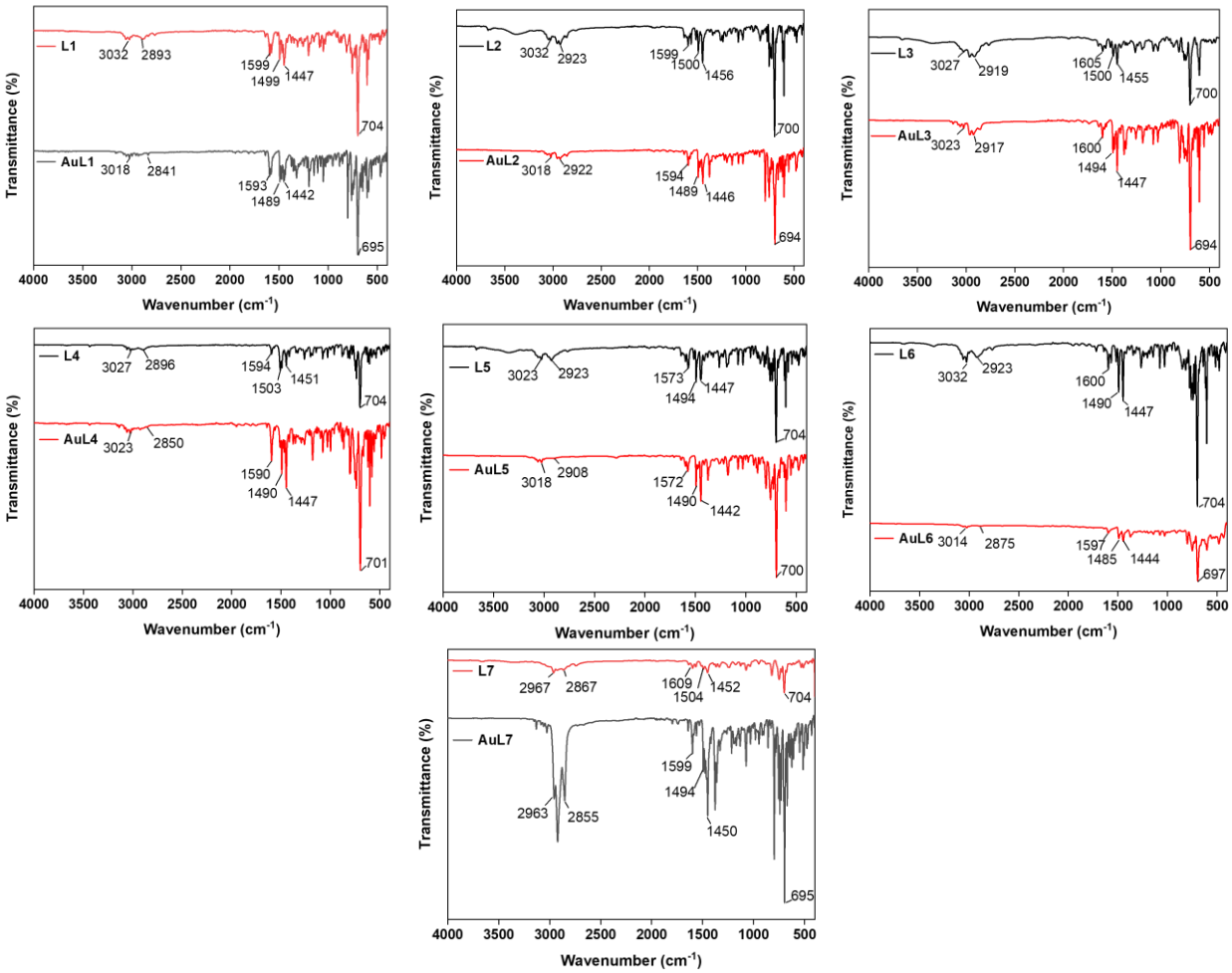


Fig S24: IR spectra of L1-L7 and AuL1-AuL 7 in solid state.

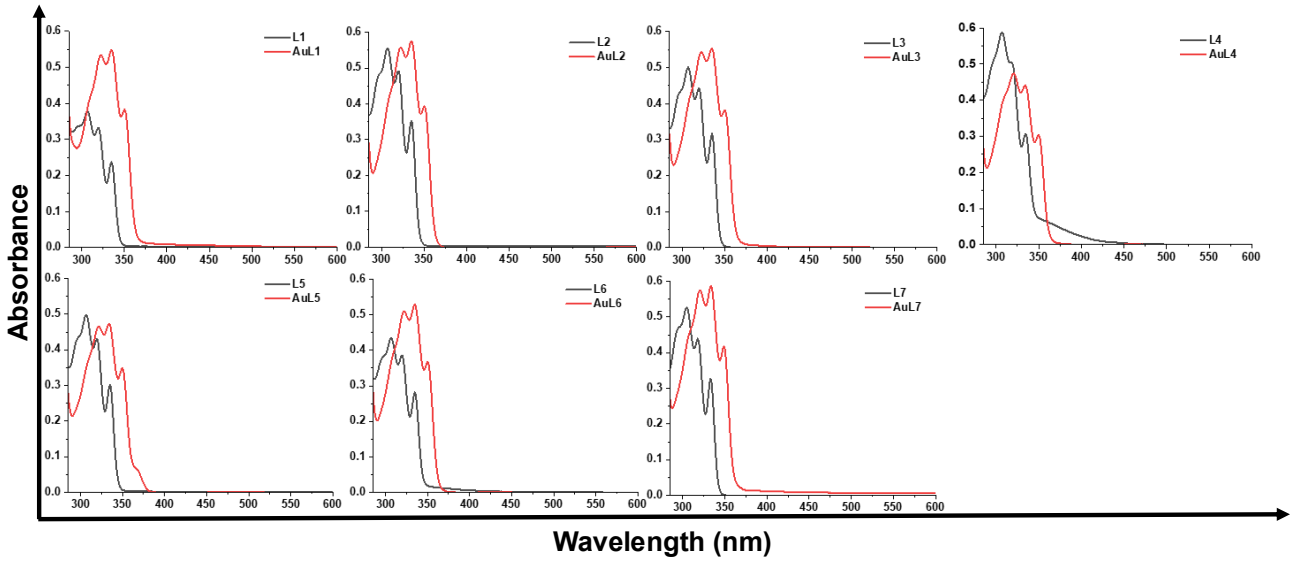


Fig S25: UV-Vis absorption spectra of L1-L7 and AuL1-AuL 7 in room temperature in DMSO.

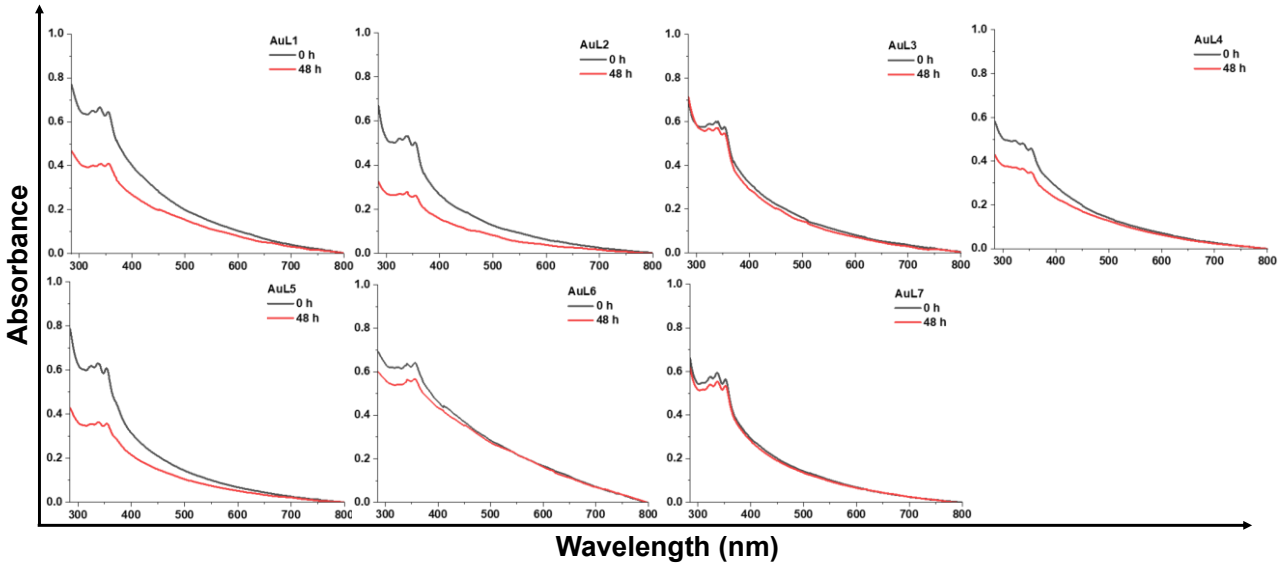


Fig S26: UV-Vis absorption spectra of AuL1-AuL7 in room temperature in 1X PBS for 48 h.

Table S3: Cartesians coordinates of AuL3 at the BP86/def2TZVP.

Atom	X	Y	Z
Au	-1.21866600	-0.04775100	-2.08968500
Cl	-0.68324300	-0.07440600	-4.31176000
N	-0.66214300	0.00707300	0.83351900
N	-2.81761600	-0.03220300	0.57004500
C	-6.53571400	-0.09298800	0.57326000
H	-7.34187900	-0.09508000	1.31047300
C	0.52583300	-2.98190800	2.00890800
C	2.82713800	-1.14181500	0.20091700
H	3.35667600	-2.08869700	0.08133400
C	0.71969600	-2.53427400	0.55852900
H	-0.29126700	-2.37530400	0.14705800
C	0.45854400	3.06353400	1.96573000
C	-1.19603600	0.01862600	2.10554000
H	-0.57786000	0.04221600	2.99379600
C	1.45109600	-1.19459700	0.43876000
C	2.79402900	1.25600000	0.18598400

H	3.28892600	2.21820500	0.05660500
C	-5.77418800	-0.11486800	-1.71313600
H	-5.98538100	-0.13434900	-2.78347700
C	2.12915800	-4.66118400	0.19500800
H	2.28473400	-4.73610400	1.27312000
C	-4.15175700	-0.06127100	0.08162900
C	-1.63191700	-0.02403100	-0.13732000
C	1.35149000	-3.61735900	-0.32478100
C	3.52791000	0.06897200	0.07834900
C	-0.66244300	3.84825900	2.28534700
H	-1.38868600	4.08557700	1.50344300
C	1.22109300	3.66162500	-0.40016300
C	1.41166000	1.26503600	0.42354600
C	1.96380200	4.75019400	0.07695300
H	2.12996500	4.86422700	1.15002600
C	2.49236700	-5.54613300	-2.03375000
H	2.93178600	-6.29530900	-2.69550200
C	-5.20396800	-0.06394000	1.04123300
C	1.22518200	-3.09983600	4.34035600
H	1.93806100	-2.82695900	5.12161900
C	1.71363800	-4.50965300	-2.56147900
H	1.54133600	-4.44301600	-3.63755400
C	2.26495400	5.57850200	-2.18260400
H	2.66671900	6.32312900	-2.87281800
C	-2.56136500	-0.00593100	1.96450800
C	-4.44894100	-0.08661100	-1.28687300
H	-3.63519700	-0.08401300	-2.01654900
C	-6.82454100	-0.11827800	-0.78414800
H	-7.86093500	-0.14051800	-1.12498900
C	-3.63142200	-0.00907800	2.90334000
H	-3.38740800	0.01147600	3.96540500
C	-0.57970600	-3.78683600	2.33162700

H	-1.28765500	-4.06211900	1.54540200
C	0.12098700	-3.89834300	4.64807200
H	-0.03608500	-4.25165900	5.66912800
C	-0.85814000	4.33003700	3.58095600
H	-1.73823300	4.93601100	3.80663400
C	2.48423500	5.70150300	-0.80885700
H	3.05871400	6.54455300	-0.41870800
C	1.18821700	3.25783300	4.28280700
H	1.91890000	3.02240900	5.05979800
C	-0.78292100	-4.24088700	3.63610100
H	-1.65077300	-4.86336300	3.86423500
C	2.69788300	-5.61822800	-0.65424000
H	3.29892700	-6.42603800	-0.23093900
C	1.14932900	-3.55463200	-1.71434500
H	0.54796000	-2.74429900	-2.13729200
C	1.42461000	-2.64482400	3.03148700
H	2.28822800	-2.01635000	2.80377900
C	-4.91437300	-0.03742600	2.45413500
H	-5.75167100	-0.04057000	3.15422200
C	0.06881200	4.03603400	4.58734600
H	-0.08234200	4.41093400	5.60156900
C	1.38020300	2.77508200	2.98274200
H	2.25609200	2.16273300	2.75810300
C	0.75834500	0.02754800	0.55646300
C	0.64052000	2.58365000	0.52406300
H	-0.37243900	2.38290100	0.13683800
C	1.52121200	4.49656400	-2.66795000
H	1.33871900	4.38963100	-3.73908900
C	1.00500100	3.54750200	-1.78434500
H	0.43079700	2.70152100	-2.17407600
C	5.04071200	0.05028800	-0.20080700
C	5.29493100	-0.65858000	-1.55296800

H	4.92564600	-1.69399100	-1.54739900
H	6.37478400	-0.68577800	-1.76798600
H	4.79379200	-0.12752200	-2.37570900
C	5.76230100	-0.72454300	0.92717500
H	5.60668600	-0.23843700	1.90263900
H	6.84549600	-0.75588200	0.73125500
H	5.40636900	-1.76203200	1.00386500
C	5.63981900	1.46627800	-0.27471800
H	5.19754800	2.05830000	-1.08964700
H	6.72125000	1.39650800	-0.46575300
H	5.50414000	2.02011800	0.66693800

Table S4: Cartesians coordinates of AuL4 at the BP86/def2TZVP.

Atom	X	Y	Z
Au	-0.00002700	1.07637100	-2.01681400
Cl	-0.00003100	0.76505000	-4.27989900
N	-0.00000400	0.23912800	0.84042600
N	-0.00007600	2.41017500	0.78414800
C	-0.00019100	6.11171600	1.14272600
H	-0.00024400	6.84356800	1.95373000
C	-3.02643400	-1.00886600	1.87722200
C	-1.21862400	-3.15223900	-0.12226300
H	-2.14811600	-3.69067600	-0.30895900
C	-2.56388800	-1.06032100	0.41946100
H	-2.38041900	-0.01639900	0.11541100
C	3.02650100	-1.00876200	1.87725000
C	-0.00004100	0.64897200	2.15839800
H	-0.00003900	-0.05101200	2.98410600
C	-1.23633900	-1.80040000	0.24174400
C	1.21879300	-3.15218600	-0.12223500
H	2.14831600	-3.69057200	-0.30891700
C	-0.00009200	5.57279100	-1.20617000

H	-0.00006100	5.88565300	-2.25148700
C	-4.69882500	-2.40006900	-0.11506400
H	-4.79045400	-2.66589600	0.93995100
C	-0.00010000	3.78550300	0.42522500
C	-0.00004300	1.29812800	-0.03375800
C	-3.64177400	-1.58290300	-0.53825900
C	0.00009900	-3.79822800	-0.28358700
C	3.81735200	0.07250200	2.30094800
H	4.06976700	0.86167500	1.58786900
C	3.64186300	-1.58268700	-0.53825100
C	1.23644000	-1.80034600	0.24176300
C	4.69893600	-2.39984800	-0.11509300
H	4.79056400	-2.66572600	0.93990900
C	-5.55287700	-2.52268600	-2.38158500
H	-6.29489100	-2.88555600	-3.09562800
C	-0.00016100	4.74096400	1.48107900
C	-3.18920600	-1.94060000	4.12286000
H	-2.93975200	-2.73465600	4.83002600
C	-4.50261800	-1.70394500	-2.81226000
H	-4.41787700	-1.42392700	-3.86405900
C	5.55300700	-2.52231800	-2.38161400
H	6.29503300	-2.88513200	-3.09567300
C	-0.00008000	2.02159900	2.14793700
C	-0.00006200	4.21253400	-0.90863700
H	-0.00000900	3.47297700	-1.71335500
C	-0.00016000	6.52937700	-0.18093300
H	-0.00018200	7.59381400	-0.42114600
C	-0.00013800	2.99714200	3.18488600
H	-0.00014300	2.65269600	4.21892700
C	-3.81736500	0.07235900	2.30087100
H	-4.06984200	0.86148100	1.58775600
C	-3.97363100	-0.85953800	4.53170200

H	-4.33929100	-0.80151800	5.55877400
C	4.28687600	0.14903600	3.61343200
H	4.89859700	0.99971200	3.92122000
C	5.64775300	-2.86825300	-1.03189700
H	6.46600100	-3.50283700	-0.68470300
C	3.18935200	-1.94059700	4.12284000
H	2.93995500	-2.73470500	4.82996800
C	-4.28688700	0.14892500	3.61335400
H	-4.89867000	0.99957200	3.92109800
C	-5.64762500	-2.86854700	-1.03184900
H	-6.46585500	-3.50313500	-0.68462500
C	-3.55591600	-1.23889900	-1.89827000
H	-2.73390000	-0.60567600	-2.24565400
C	-2.71901500	-2.01361000	2.80624100
H	-2.10382300	-2.86270300	2.50089000
C	-0.00018400	4.31728500	2.85993300
H	-0.00023300	5.08385600	3.63681600
C	3.97369800	-0.85949600	4.53173000
H	4.33936100	-0.80149900	5.55880200
C	2.71916300	-2.01357700	2.80621900
H	2.10402900	-2.86269800	2.50082600
C	0.00003300	-1.14748200	0.42962400
C	2.56395300	-1.06019300	0.41949200
H	2.38042100	-0.01627200	0.11547100
C	4.50273600	-1.70357200	-2.81224900
H	4.41799800	-1.42349600	-3.86403300
C	3.55601500	-1.23859900	-1.89824000
H	2.73399300	-0.60536900	-2.24559400
F	0.00013200	-5.11002400	-0.63016800

Table S5: Cartesians coordinates of AuL7 at the BP86/def2TZVP.

Atom	X	Y	Z
Au	1.70974900	-1.38953500	-0.54671400
Cl	1.02934300	-3.42596600	-1.32942000
N	1.34553800	1.32856700	0.60151200
N	3.47154100	1.03280500	0.27426400
C	2.24612200	0.40505900	0.14001300
C	4.76574500	0.54390600	-0.04845900
C	1.95605600	2.49575900	1.01273300
H	1.39589200	3.33531500	1.40535000
C	-2.84349000	0.68112600	0.75477100
C	-0.64307300	0.56450100	1.83037900
C	0.19652700	0.17475500	3.04182300
H	1.24465700	0.43290500	2.82686700
C	-2.02734400	0.36469700	1.84831600
H	-2.48697000	-0.07200200	2.73905000
C	3.30590700	2.33216000	0.81453000
C	-5.82715900	-1.63128300	1.24812300
H	-6.50149600	-0.95772900	1.78439800
C	4.97269700	-0.73511900	-0.58040700
H	4.11645900	-1.39084100	-0.75856500
C	-0.08504000	1.10757900	0.65368700
C	7.16748300	0.93757500	-0.12659600
H	8.01608800	1.60084400	0.05583400
C	4.43004900	3.17607700	1.04319800
H	4.25830700	4.16880100	1.45965000
C	-2.24823300	1.23174200	-0.38252400
H	-2.87695800	1.49279800	-1.23586900
C	0.14359700	-1.34506800	3.29051000
H	-0.87743900	-1.67416400	3.53702900
H	0.79763800	-1.61619200	4.13343300
H	0.47386700	-1.90415000	2.40308500

C	-4.64222300	-1.12065100	0.69153000
C	-0.27162200	2.04545000	-1.73860400
H	0.81726100	2.12699300	-1.60088400
C	-0.22146800	0.96064500	4.29941500
H	-0.15884000	2.04734000	4.13783100
H	0.43308200	0.70211800	5.14569100
H	-1.25532100	0.72476600	4.59464300
C	-0.86574200	1.45648400	-0.46441500
C	7.36675200	-0.33051000	-0.65430400
H	8.37469600	-0.67473300	-0.89152200
C	5.87362900	1.40660100	0.18873800
C	5.67612500	2.72520100	0.73814300
H	6.55303700	3.35355000	0.90395900
C	-4.34133500	0.37524900	0.83725700
H	-4.64977700	0.64974000	1.86205800
C	6.26264600	-1.16530600	-0.87958200
H	6.40377700	-2.16499200	-1.29351900
C	-6.15514400	-2.98224500	1.12191300
H	-7.07874900	-3.35989100	1.56605300
C	-5.29993200	-3.85046200	0.43370200
H	-5.55156800	-4.90858500	0.33806500
C	-5.18268200	1.24147400	-0.10178100
C	-3.79109300	-2.00034100	0.00805100
H	-2.85433500	-1.63476000	-0.41655700
C	-4.11789300	-3.35533200	-0.12133700
H	-3.43494200	-4.02244200	-0.65079900
C	-0.81085000	3.46393600	-2.00743200
H	-1.89789400	3.45357400	-2.17860400
H	-0.33458700	3.88899800	-2.90416100
H	-0.61182700	4.13955100	-1.16189100
C	-5.56214600	2.53077900	0.30579600
H	-5.26830900	2.88676200	1.29729900

C	-5.57584800	0.80191500	-1.37447000
H	-5.30823600	-0.20489100	-1.70180700
C	-6.31882600	1.63261200	-2.22013600
H	-6.61672600	1.27070600	-3.20656200
C	-6.30829400	3.36118000	-0.53380700
H	-6.59875800	4.35752900	-0.19352100
C	-6.68790600	2.91460300	-1.80384300
H	-7.27456700	3.55946200	-2.46114400
C	-0.50834500	1.12048700	-2.94783500
H	-0.09646500	0.11700900	-2.76667200
H	-0.02346500	1.53575300	-3.84456300
H	-1.58194400	1.01449400	-3.16610400

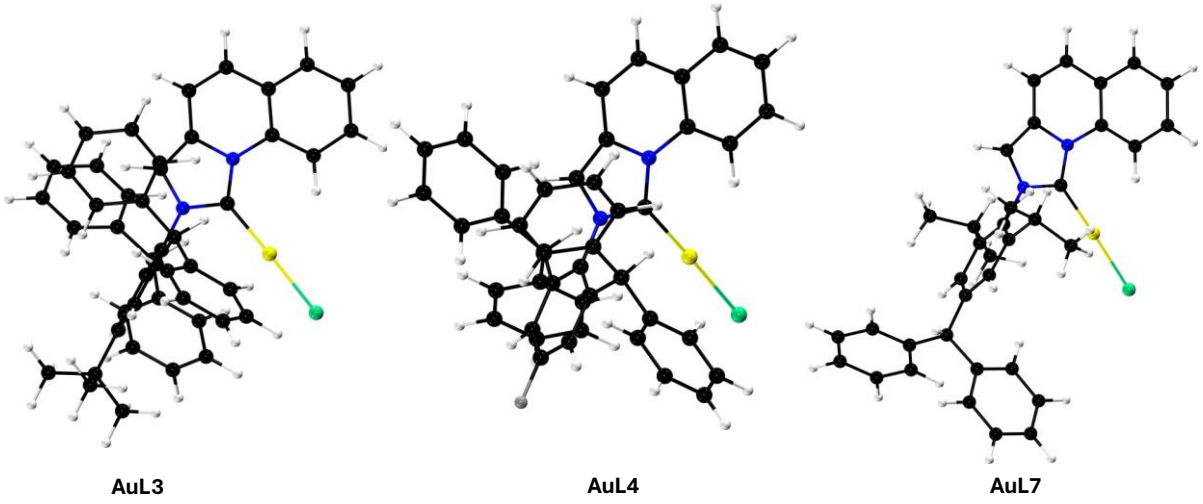


Fig S27: Optimized structures of AuL3, AuL4, AuL7 (Atom colours: Au- yellow, C- black, Cl- green, F-grey, H- white).

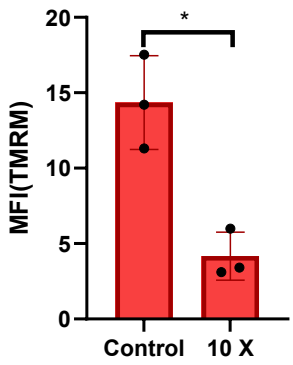


Fig S28: Mean Fluorescence Intensity of TMRM dye in A549 cells.

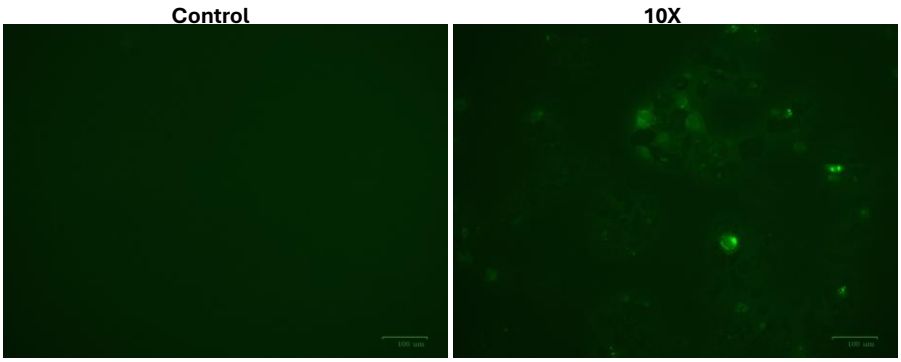


FIG S29: ROS generation in A549 cells. Cells were treated with AuL4 for 12 h and then stained with H_2DCFDA. Scale Bar :100 µm.

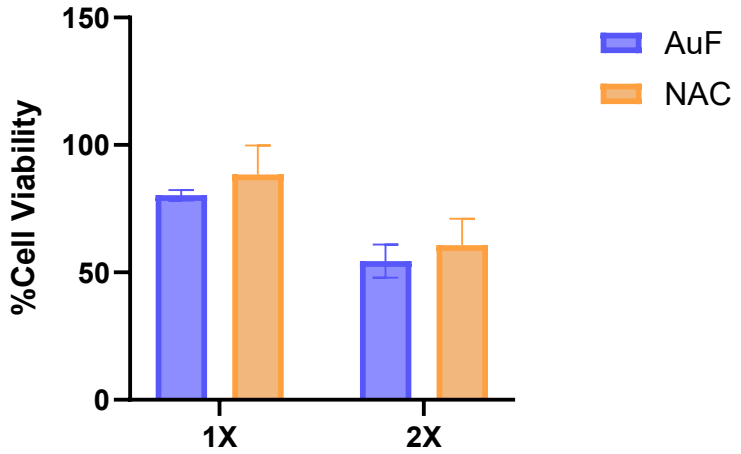


FIG S30: ROS generation in A549 cells. Relative cell viabilities in presence of ROS scavenger 2mM NAC. Cells were pretreated with NAC for 1 h and then treated with AuL4 for 24h.

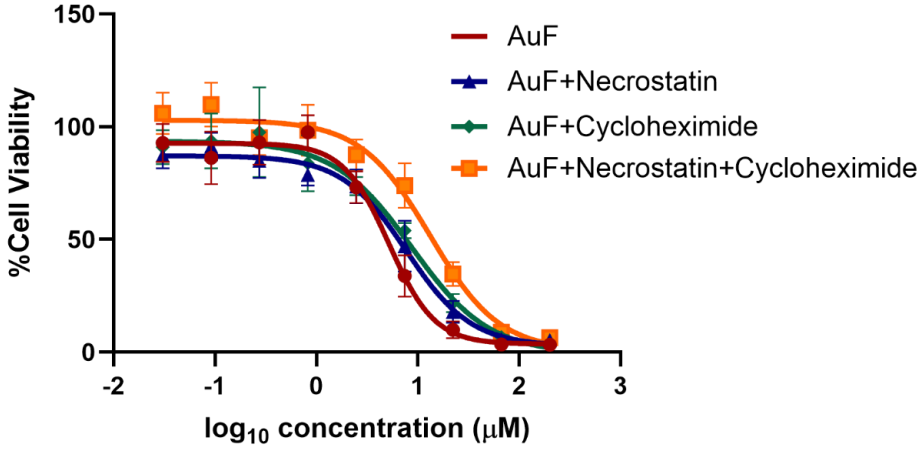


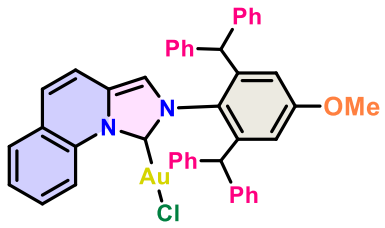
FIG S31: IC_{50} value of AuL4 in presence of inhibitor of necrostatin 1, cycloheximide, and both necrostatin and cycloheximide

Table S6: Lipophilicity of compound L1 to L7

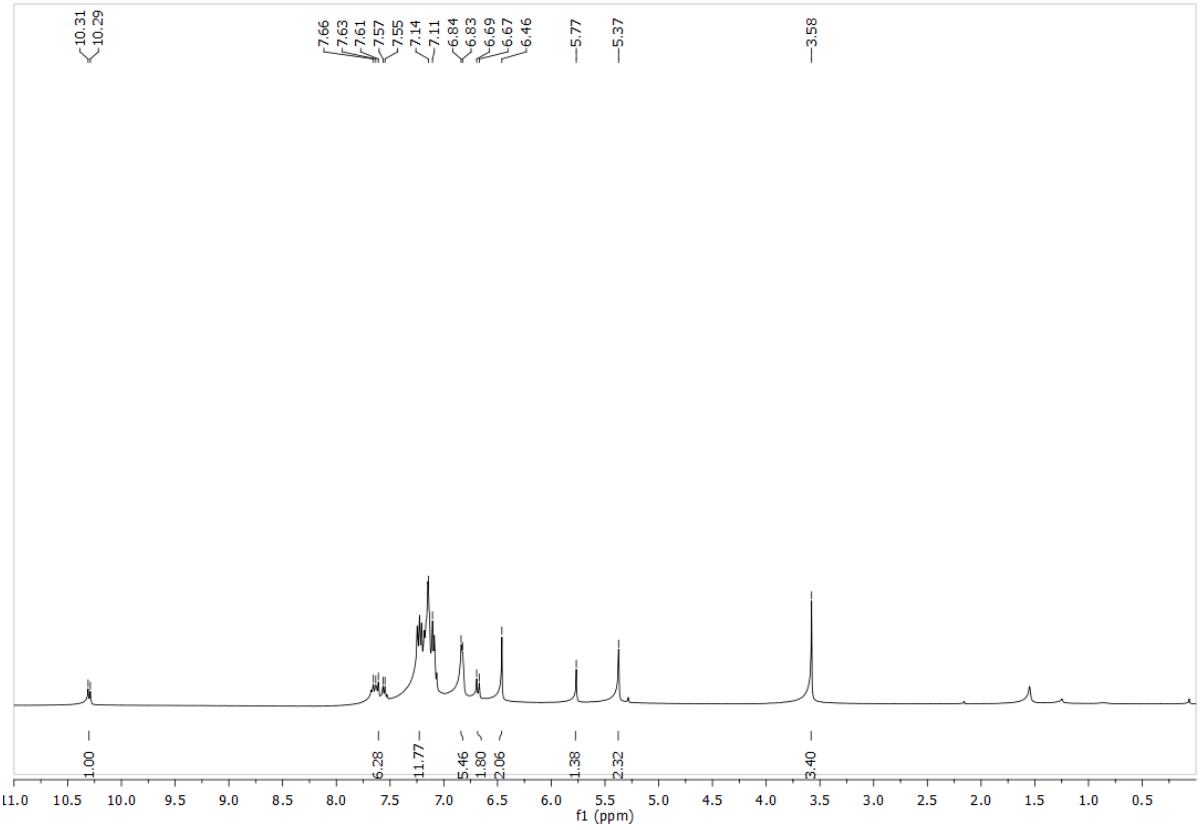
Compound	clogP
L1	5.4
L2	6.7
L3	6.8
L4	5.2
L5	5.7
L6	5.9
L7	8.5

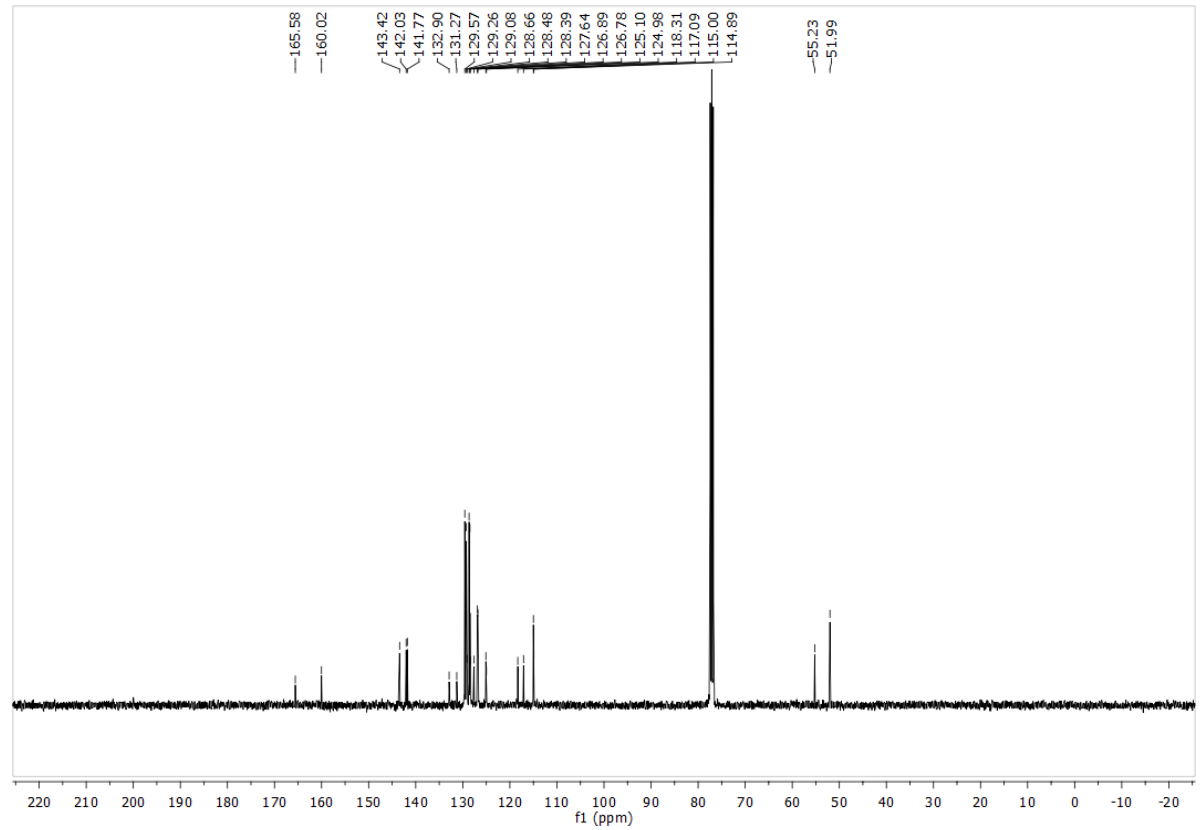
^{1}H, ^{13}C and HMBC spectra in $CDCl_3$

AuL1:



^{1}H NMR (400 MHz, CHLOROFORM-D) δ 10.30 (d, *J* = 8.4 Hz, 1H), 7.74 – 7.49 (m, 6H), 7.12 (m, 12 H), 6.83 (d, *J* = 5.3 Hz, 5H), 6.68 (d, *J* = 9.5 Hz, 2H), 6.46 (s, 2H), 5.77 (s, 1H), 5.37 (s, 2H), 3.58 (s, 3H). ^{13}C NMR (100 MHz, CHLOROFORM-D) δ 165.58, 160.02, 143.42, 142.03, 141.77, 132.90, 131.27, 129.57, 129.26, 129.08, 128.66, 128.48, 128.39, 127.64, 126.89, 126.78, 125.10, 124.98, 118.31, 117.09, 115.00, 114.89, 55.23, 51.99.


10.31
10.29
7.66
7.63
7.61
7.57
7.55
7.14
7.11
6.84
6.83
6.69
6.67
6.46
5.77
5.37
3.58
1.00
6.28
11.77
5.46
1.80
2.06
1.38
2.32
3.40
f1 (ppm)


165.58
160.02
143.42
142.03
141.77
132.90
131.27
129.57
129.26
129.08
128.66
128.48
128.39
127.64
126.89
126.78
125.10
124.98
118.31
117.09
115.00
114.89
55.23
51.99
f1 (ppm)

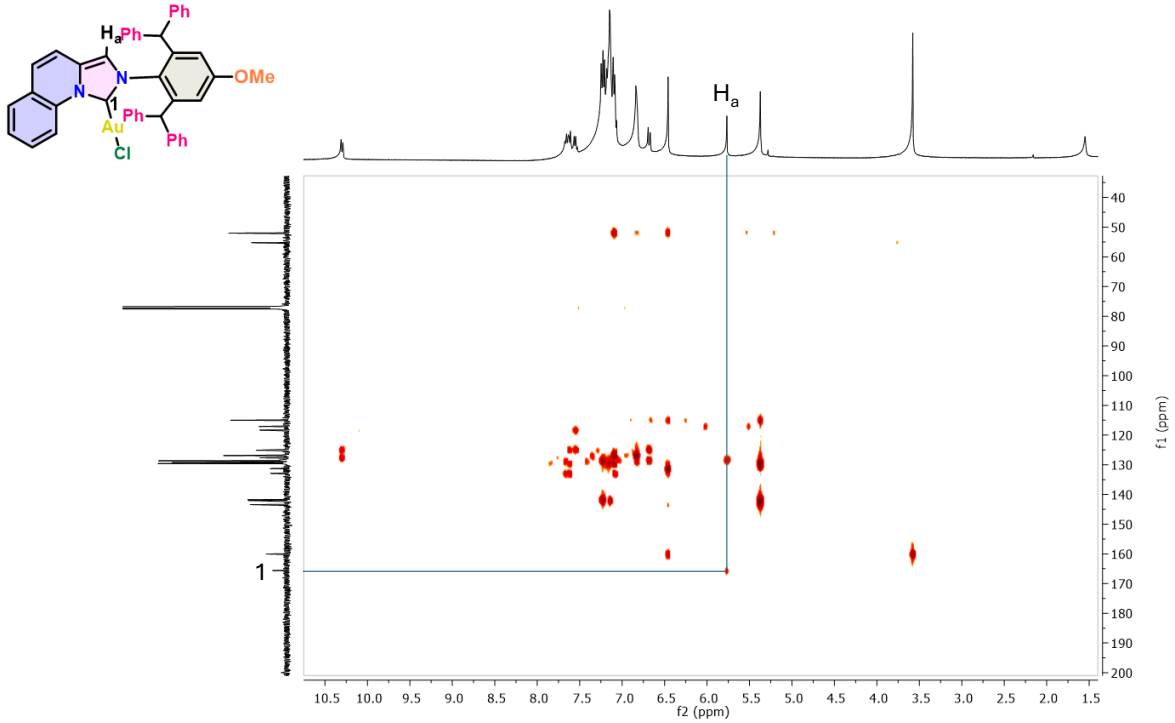
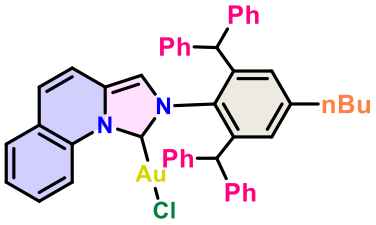
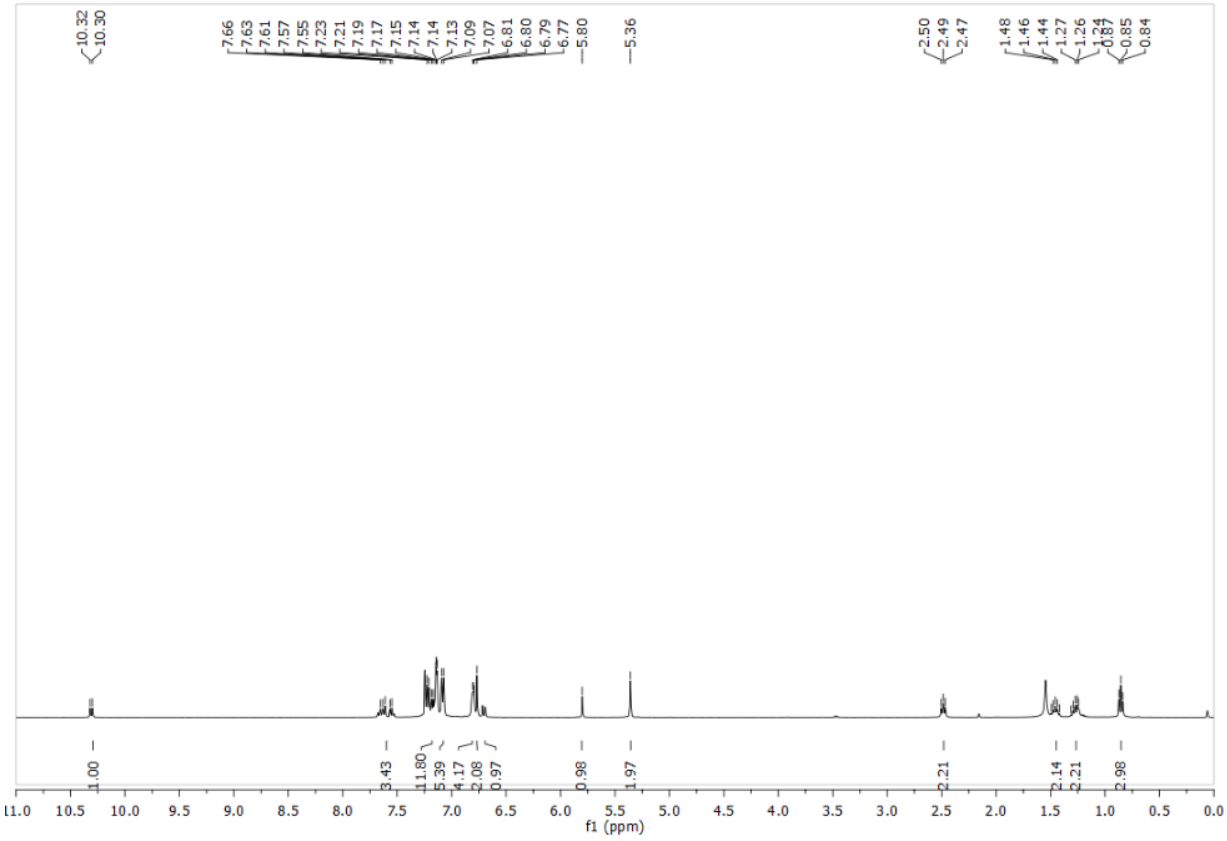


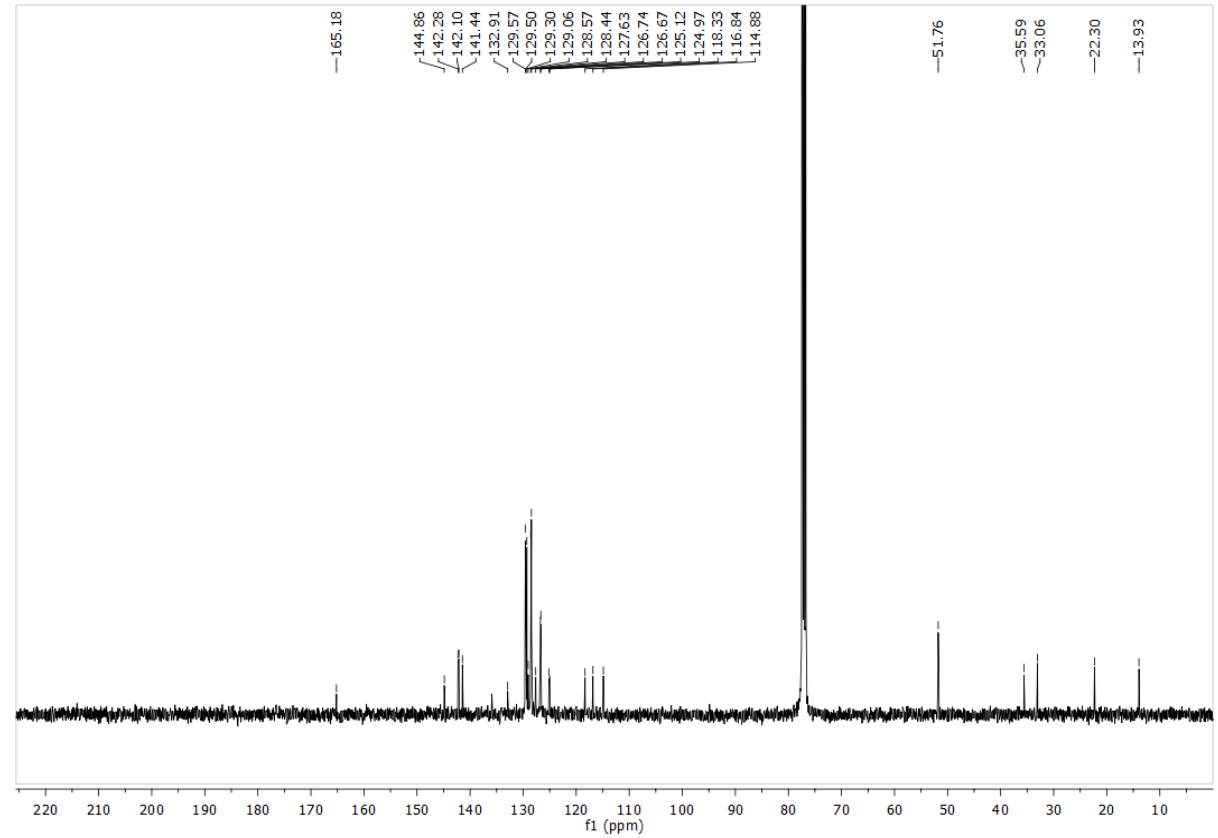
FIG S32 ^{1}H, ^{13}C and HMBC spectra in $CDCl_3$ of AuL1

AuL2:



^{1}H NMR (400 MHz, CHLOROFORM-D) δ 10.31 (d, *J* = 8.5 Hz, 1H), 7.68 – 7.53 (m, 3H), 7.26 – 7.12 (m, 12H), 7.08 (d, *J* = 7.2 Hz, 5H), 6.83 – 6.79 (m, 4H), 6.77 (s, 2H), 6.70 (d, *J* = 9.5 Hz, 1H), 5.80 (s, 1H), 5.36 (s, 2H), 2.56 – 2.38 (m, 2H), 1.46 (m, 2H), 1.28 (m, 2H), 0.85 (t, *J* = 7.2 Hz, 3H). ^{13}C NMR (100 MHz, CHLOROFORM-D) δ 165.18, 144.86, 142.28, 142.10, 141.44, 132.91, 129.57, 129.50, 129.30, 129.06, 128.57, 128.44, 127.63, 126.74, 126.67, 125.12, 124.97, 118.33, 116.84, 114.88, 51.76, 35.59, 33.06, 22.30, 13.93.


10.32
10.30
7.66
7.63
7.61
7.57
7.55
7.23
7.21
7.19
7.17
7.15
7.14
7.14
7.13
7.09
7.07
6.81
6.80
6.79
6.77
5.80
5.36
2.50
2.49
2.47
1.48
1.46
1.44
1.27
1.26
1.24
0.87
0.85
0.84
1.00
3.43
11.80
5.39
4.17
2.08
0.97
0.98
1.97
2.21
2.14
2.21
2.98
f1 (ppm)


165.18
144.86
142.28
142.10
141.44
132.91
129.57
129.50
129.30
129.06
128.57
128.44
127.63
126.74
126.67
125.12
124.97
118.33
116.84
114.88
51.76
35.59
33.06
22.30
13.93
f1 (ppm)

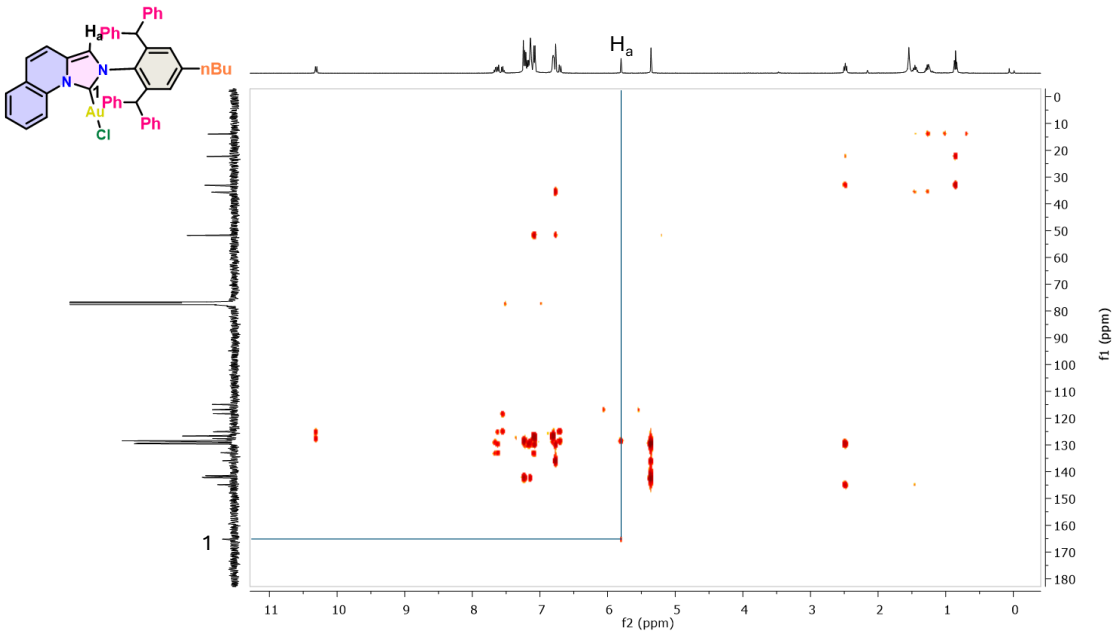
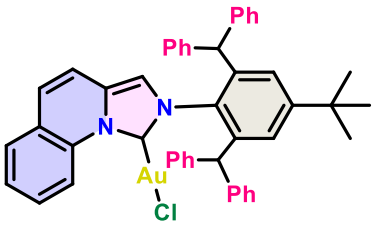
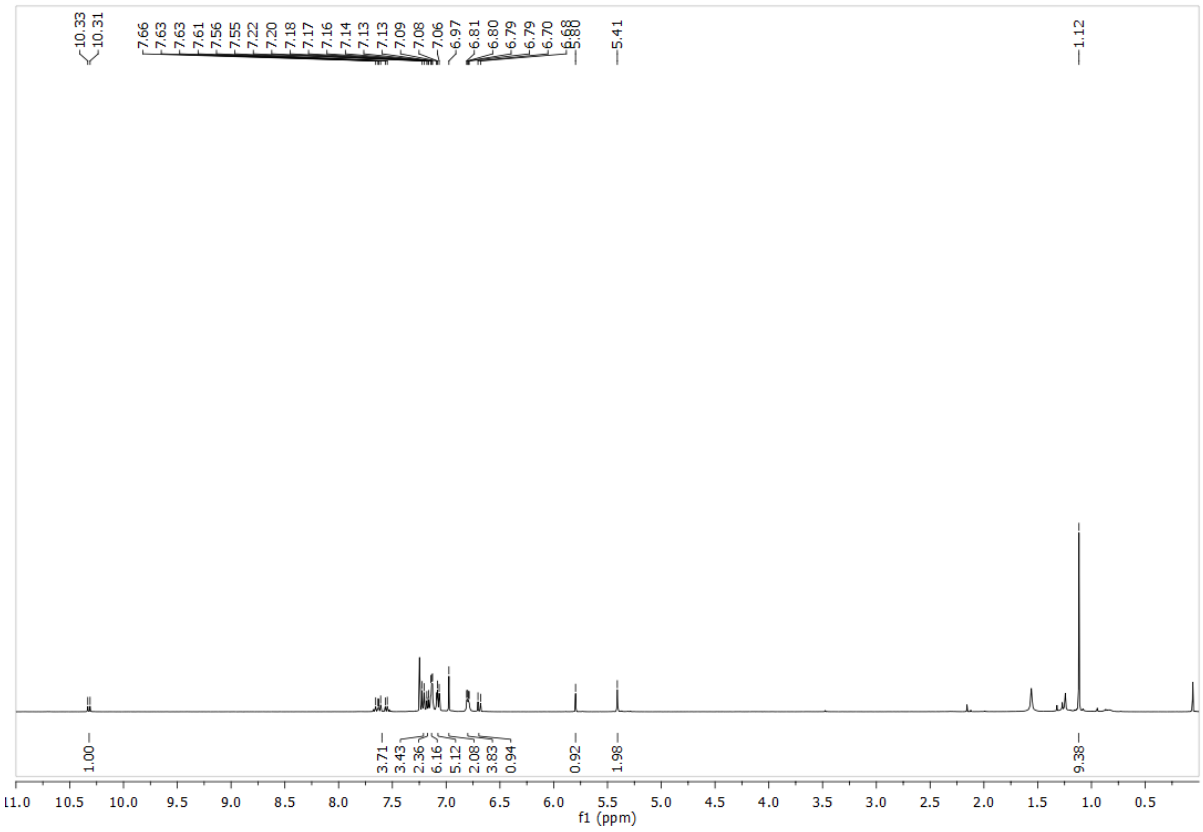


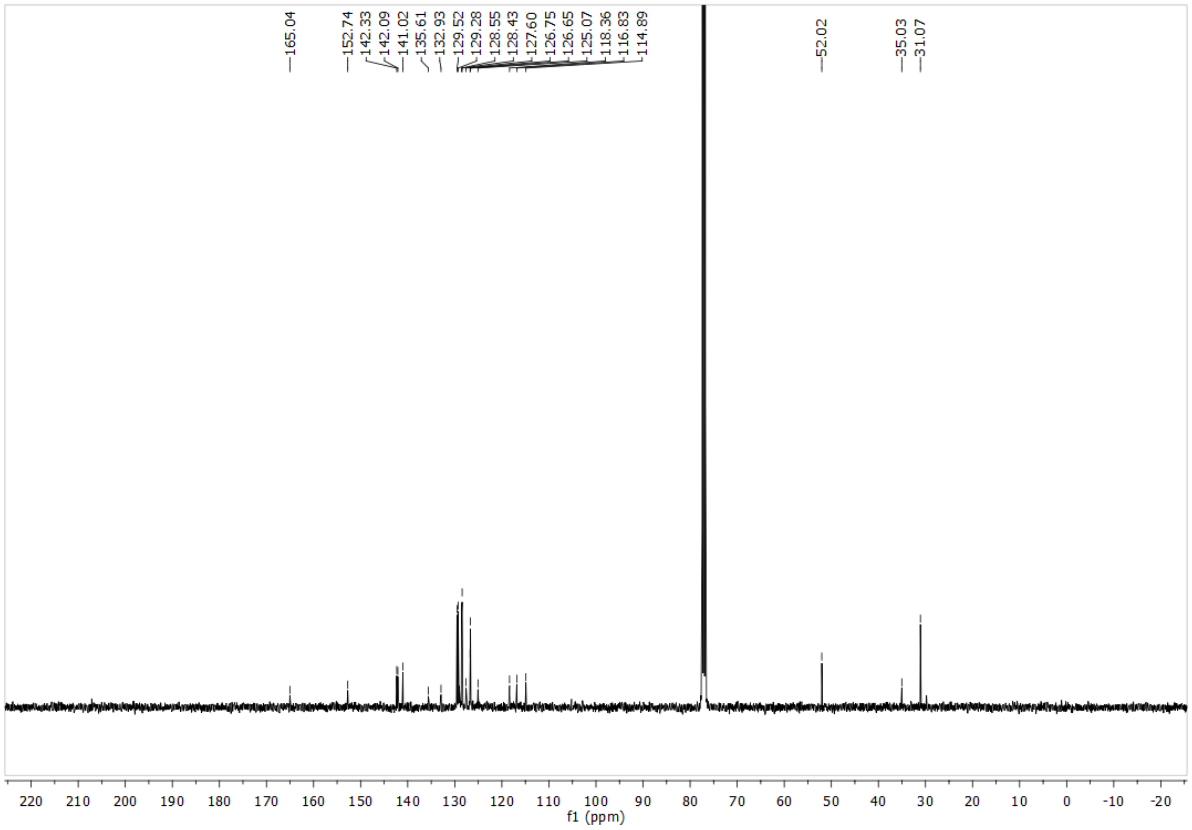
FIG S33 ^{1}H, ^{13}C and HMBC spectra in $CDCl_3$ of AuL2

AuL3:



^{1}H NMR (400 MHz, CHLOROFORM-D) δ 10.32 (d, *J* = 8.5 Hz, 1H), 7.67 – 7.53 (m, 4H), 7.21 (d, *J* = 7.6 Hz, 3H), 7.19 – 7.16 (m, 2H), 7.15 – 7.12 (m, 6H), 7.08 (t, *J* = 5.0 Hz, 5H), 6.97 (s, 2H), 6.80 (dd, *J* = 6.3, 3.2 Hz, 4H), 6.69 (d, *J* = 9.5 Hz, 1H), 5.80 (s, 1H), 5.41 (s, 2H), 1.12 (s, 9H). ^{13}C NMR (100 MHz, CHLOROFORM-D) δ 165.04, 152.74, 142.33, 142.09, 141.02, 135.61, 132.93, 129.52, 129.28, 128.55, 128.43, 127.60, 126.75, 126.65, 125.07, 118.36, 116.83, 114.89, 52.02, 35.03, 31.07.


10.33
10.31
7.66
7.63
7.63
7.61
7.56
7.55
7.22
7.20
7.18
7.17
7.16
7.14
7.13
7.13
7.09
7.08
7.06
6.97
6.81
6.80
6.79
6.79
6.70
6.68
6.68
5.80
5.41
1.12
1.00
3.71
3.43
2.36
6.16
5.12
2.08
3.83
0.94
0.92
1.98
9.38
f1 (ppm)


165.04
152.74
142.33
142.09
141.02
135.61
132.93
129.52
129.28
128.55
128.43
127.60
126.75
126.65
125.07
118.36
116.83
114.89
52.02
35.03
31.07
f1 (ppm)

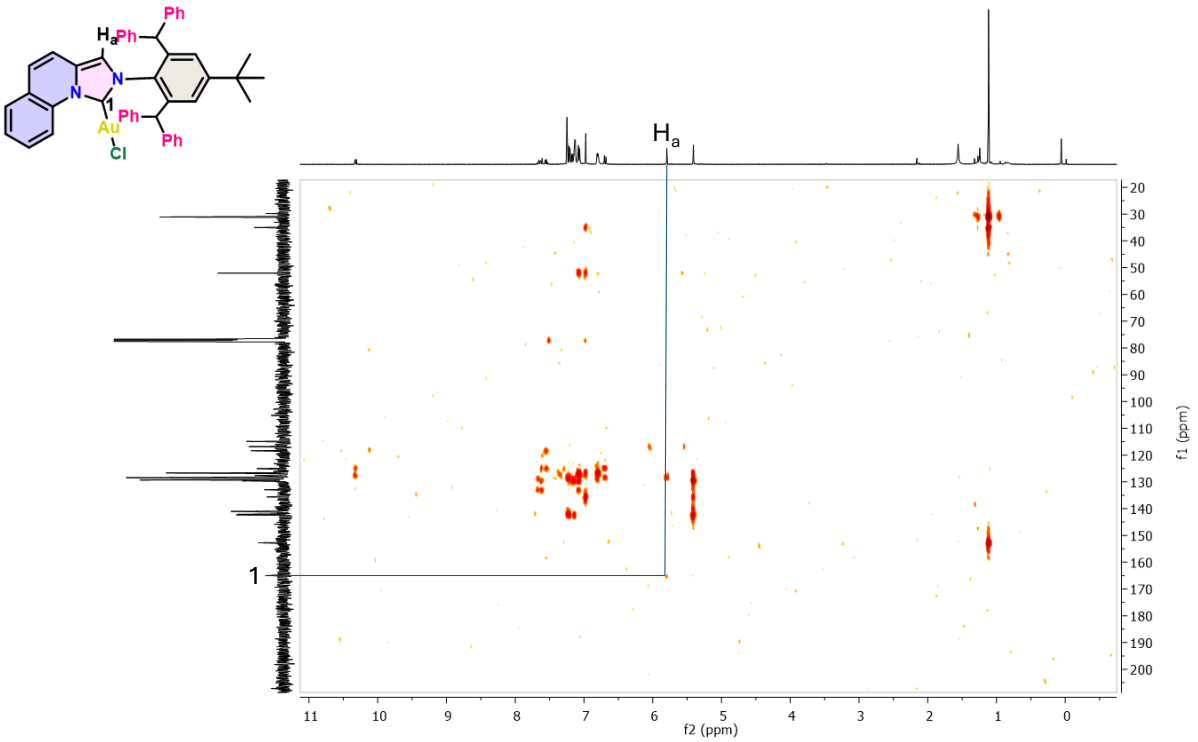
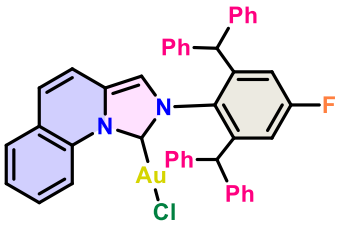


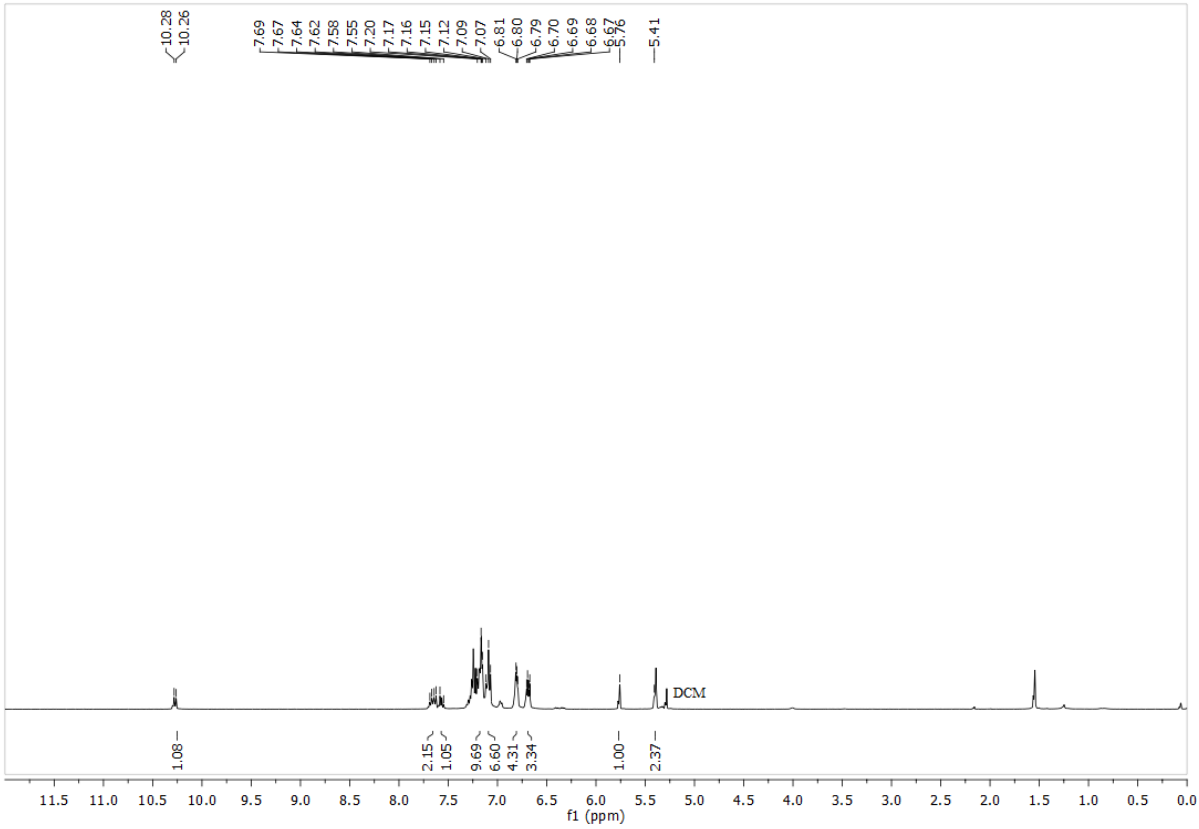
FIG S34 ^{1}H, ^{13}C and HMBC spectra in $CDCl_3$ of AuL3

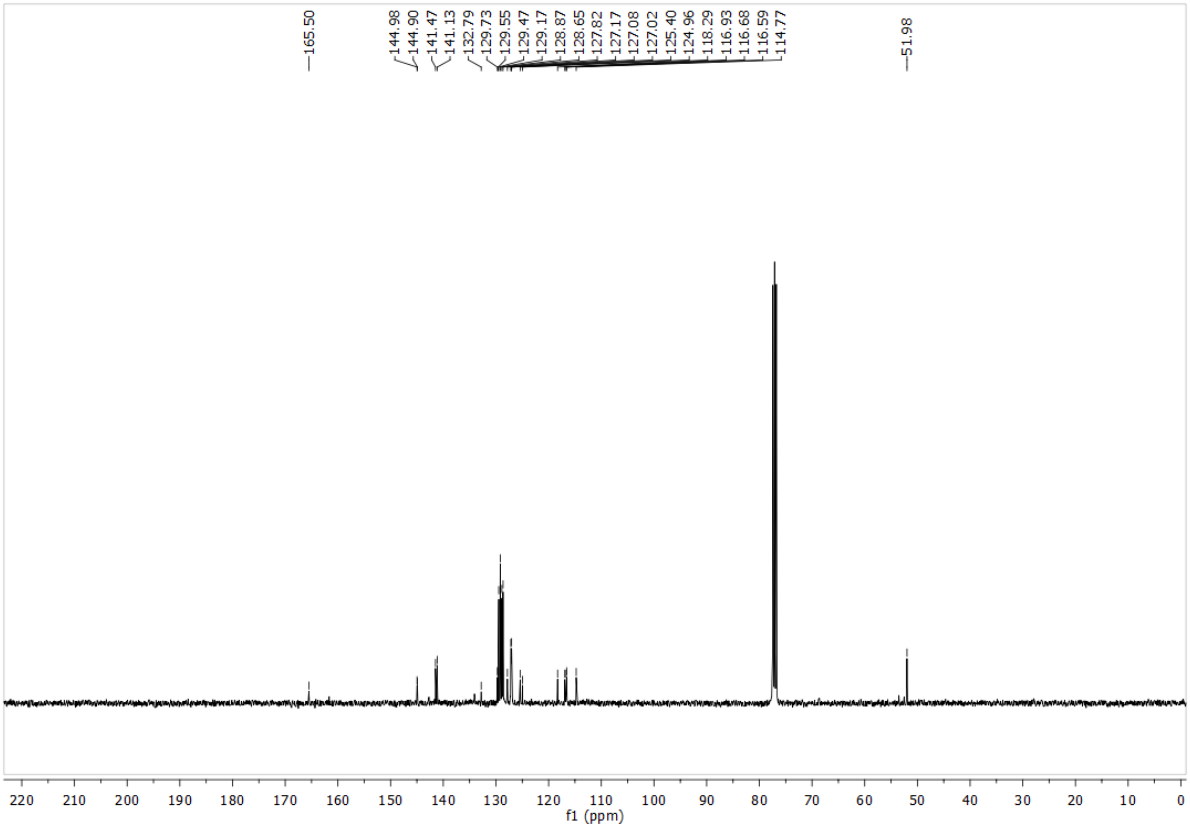
AuL4:



^{1}H NMR (400 MHz, CHLOROFORM-D) δ 10.27 (d, *J* = 8.2 Hz, 1H), 7.63 (dt, *J* = 30.7, 11.0 Hz, 3H), 7.17 (m, 10H), 7.09 (m, 7H), 6.89 – 6.78 (m, 4H), 6.69 (dd, *J* = 9.2, 3.4 Hz, 3H), 5.76 (s, 1H), 5.41 (s, 2H).^{13}C NMR (*δ* ppm CHLOROFORM-D, 100 MHz, proton decoupled): 165.50, 144.98, 144.90, 141.47, 141.13, 132.79, 129.73, 129.55, 129.47, 129.17, 128.87,

128.65, 127.82, 127.17, 127.08, 127.02, 125.40, 124.96, 118.29, 116.93, 116.68, 116.59, 114.77, 51.98.





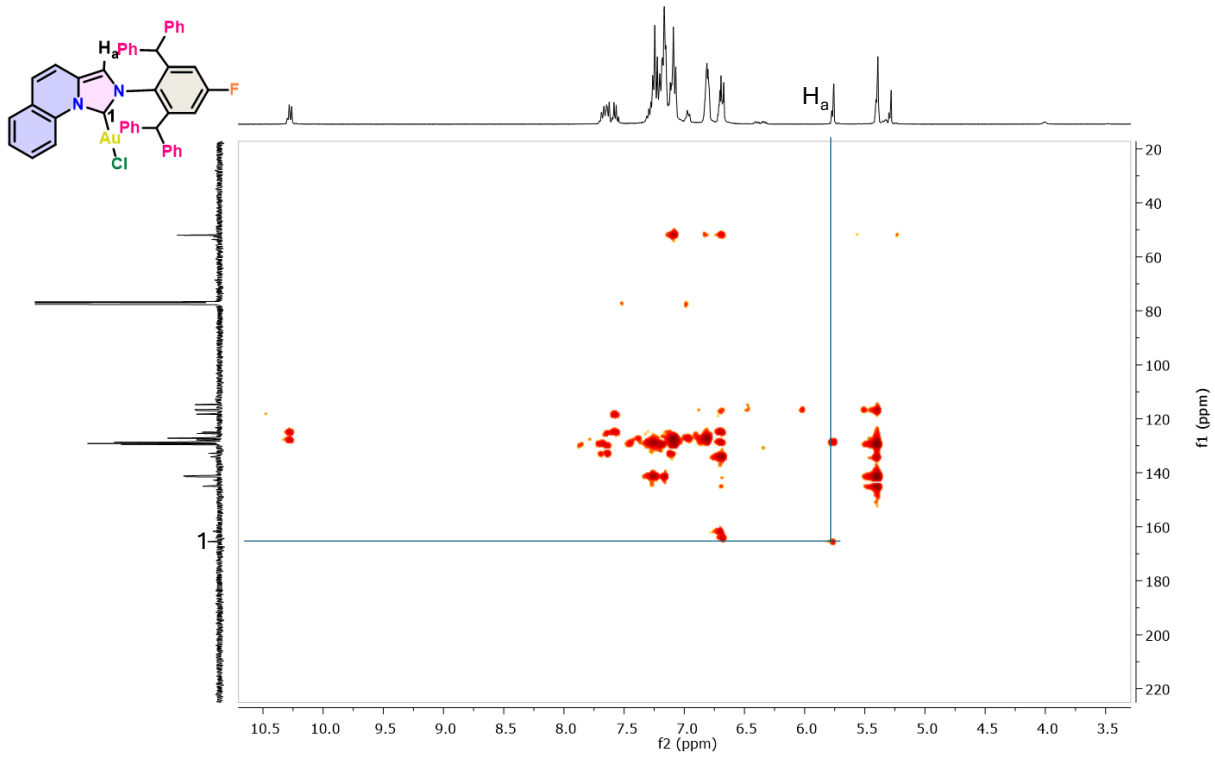
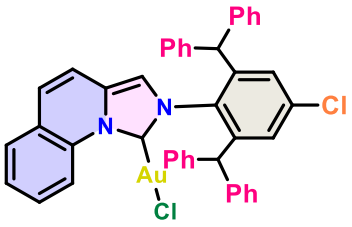


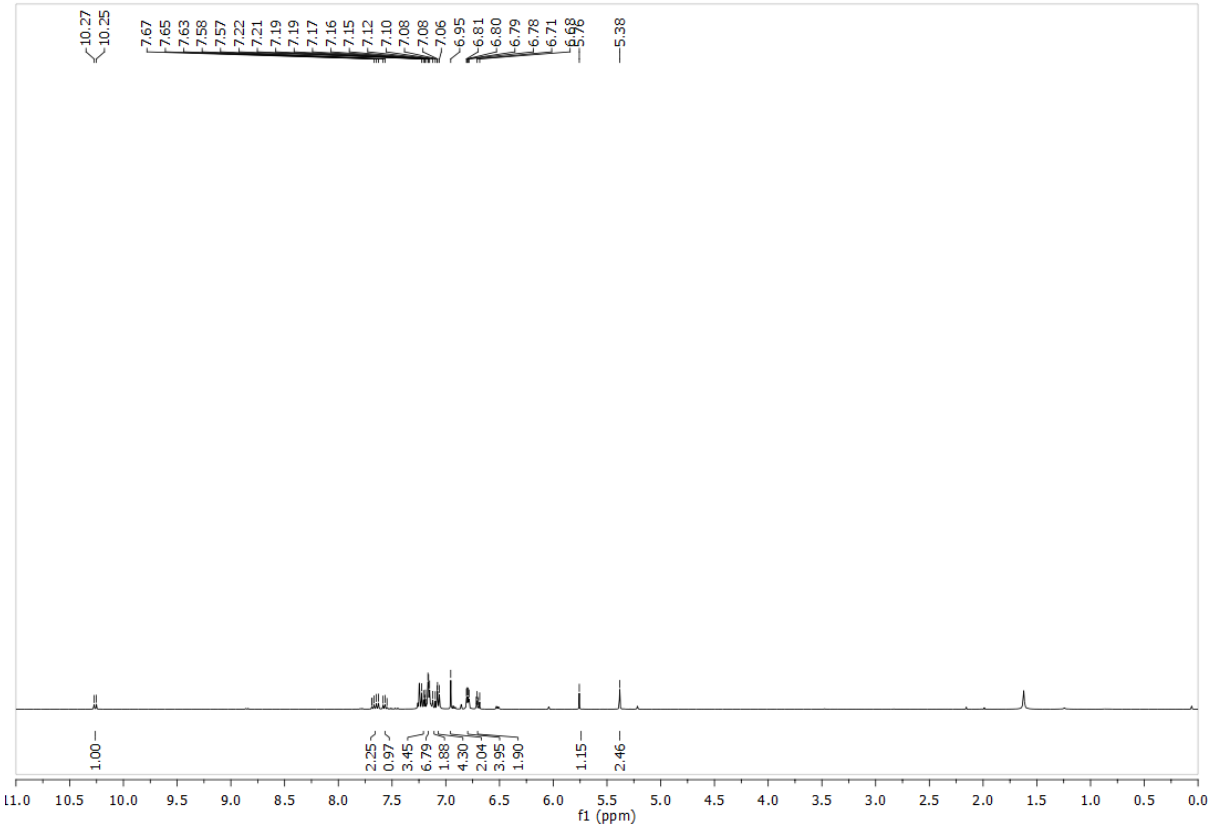
FIG S35 ^{1}H, ^{13}C and HMBC spectra in $CDCl_3$ of AuL4

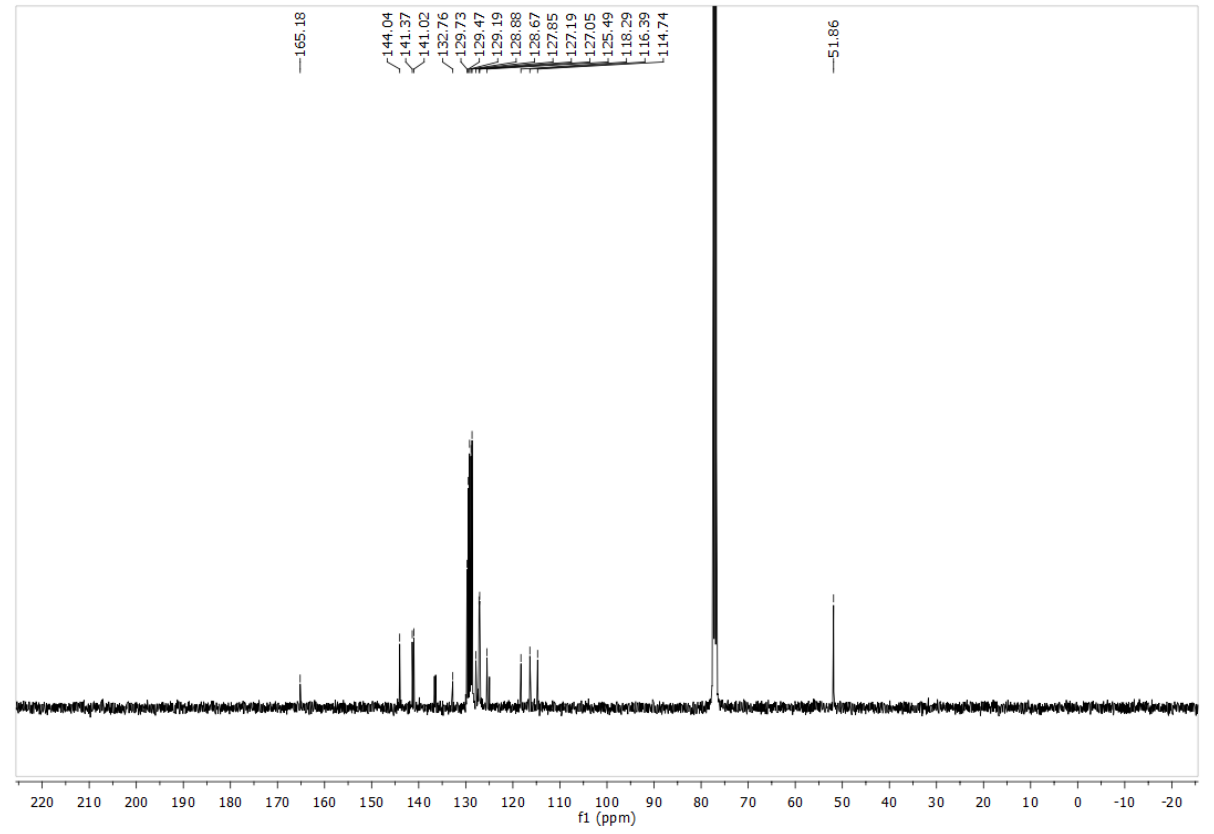
AuL5:



^{1}H NMR (396 MHz, CHLOROFORM-D) δ 10.26 (d, *J* = 8.4 Hz, 1H), 7.66 (dd, *J* = 16.0, 7.5 Hz, 2H), 7.57 (t, *J* = 7.3 Hz, 1H), 7.20 (dd, *J* = 9.3, 4.7 Hz, 3H), 7.18 – 7.13 (m, 7H), 7.11 (d, *J* = 9.4 Hz, 2H), 7.08 – 7.05 (m, 4H), 6.95 (s, 2H), 6.80 (dd, *J* = 6.5, 2.8 Hz, 4H), 6.70 (dd, *J* = 8.5, 3.9 Hz, 2H), 5.76 (s, 1H), 5.38 (s, 2H). ^{13}C NMR (100 MHz, CHLOROFORM-D) δ 165.18, 144.04, 141.37, 141.02, 132.76, 129.73, 129.47, 129.19, 128.88, 128.67, 127.85, 127.19,

127.05, 125.49, 118.29, 116.39, 114.74, 51.86.





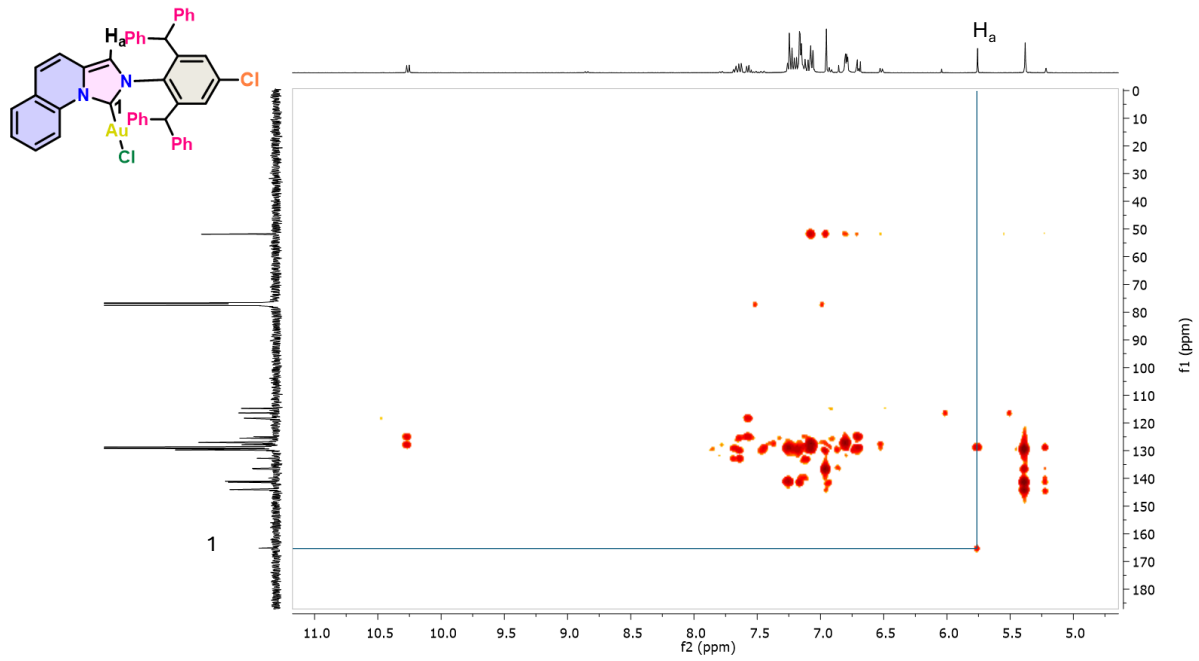
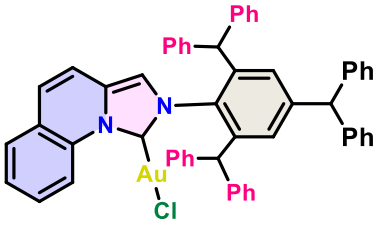
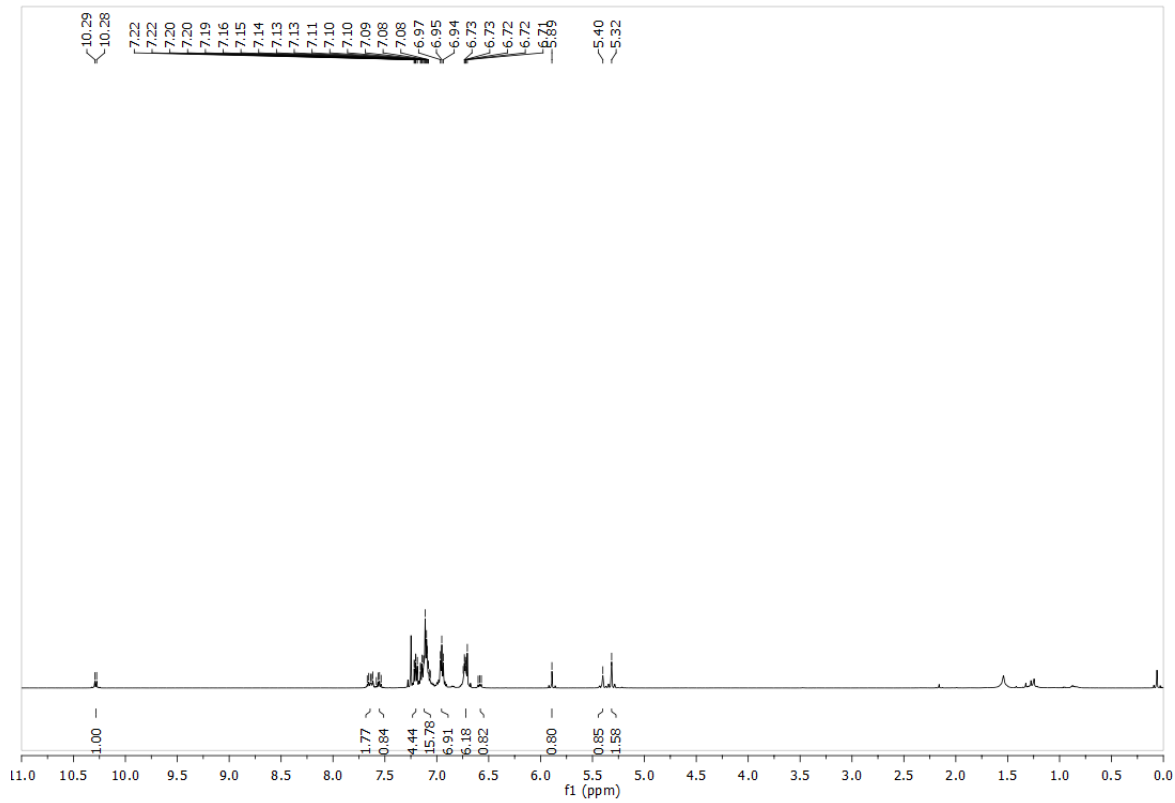


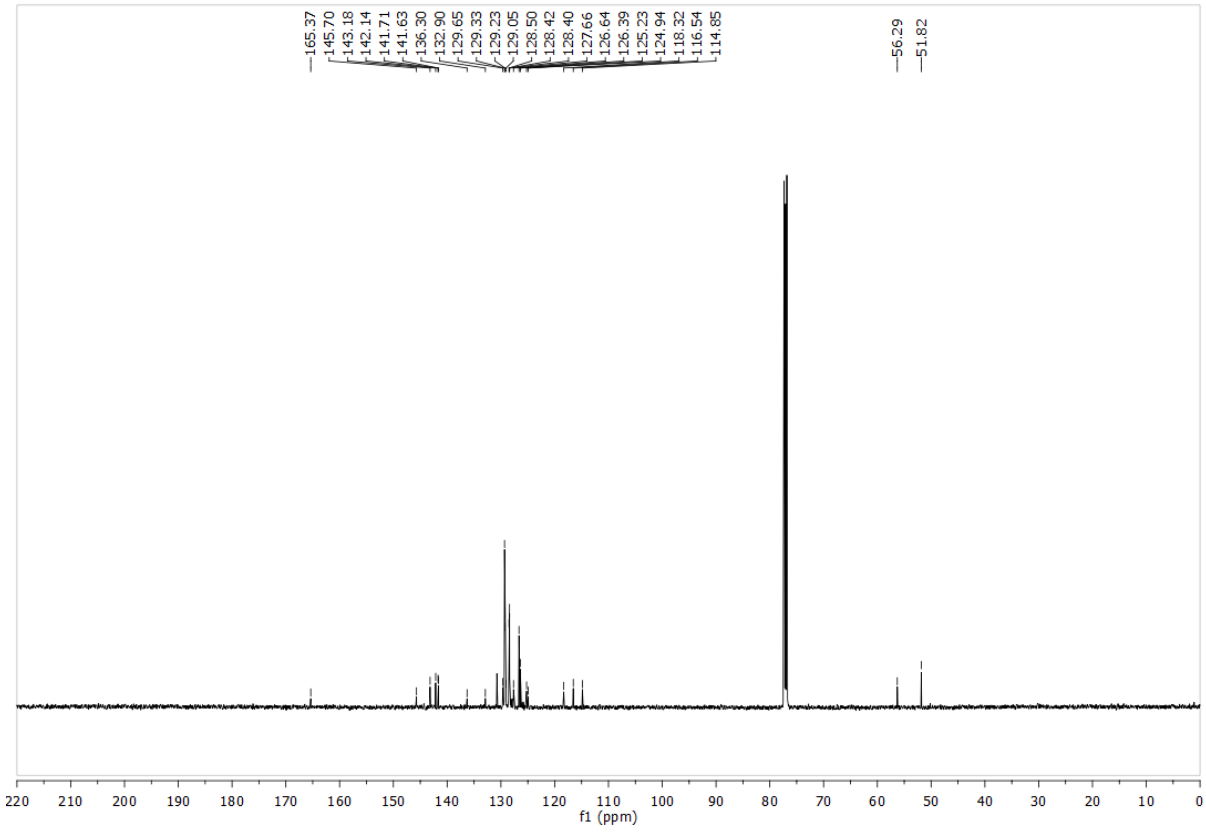
FIG S36 ^{1}H, ^{13}C and HMBC spectra in $CDCl_3$ of AuL5

AuL6:



^{1}H NMR (400 MHz, CHLOROFORM-D) δ 10.29 (d, *J* = 8.5 Hz, 1H), 7.63 (dd, *J* = 12.1, 8.1 Hz, 2H), 7.58 – 7.52 (m, 1H), 7.23 – 7.19 (m, 4H), 7.16 – 7.06 (m, 16H), 6.95 (t, *J* = 7.1 Hz, 7H), 6.75 – 6.70 (m, 6H), 6.58 (d, *J* = 7.4 Hz,1H), 5.89 (s,1H), 5.40 (s,1H), 5.32 (s,2H). NMR (126 MHz,) δ 165.37, 145.70, 143.18, 142.14, 141.71, 141.63, 136.30, 132.90, 129.65, 129.33, 129.23, 129.05, 128.50, 128.42, 128.40, 127.66, 126.64, 126.39, 125.23, 124.94, 118.32, 116.54, 114.85, 56.29, 51.82.


10.29
10.28
7.22
7.22
7.20
7.20
7.19
7.16
7.15
7.14
7.13
7.13
7.11
7.10
7.10
7.09
7.08
7.08
6.97
6.95
6.94
6.73
6.73
6.72
6.72
5.40
5.32
1.00
1.77
0.84
4.44
15.78
6.91
6.18
0.82
0.80
0.85
1.58
f1 (ppm)


165.37
145.70
143.18
142.14
141.71
141.63
136.30
132.90
129.65
129.33
129.23
129.05
128.50
128.42
128.40
127.66
126.64
126.39
125.23
124.94
118.32
116.54
114.85
56.29
51.82
f1 (ppm)

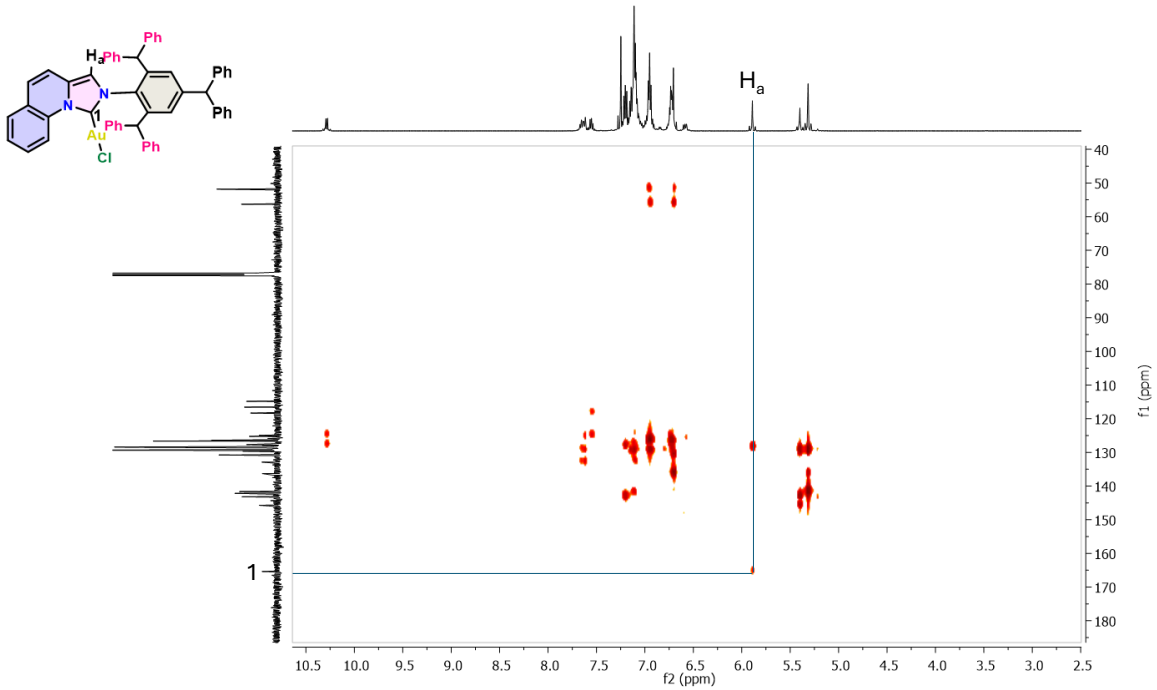
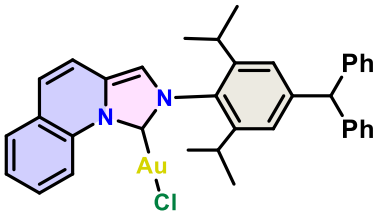
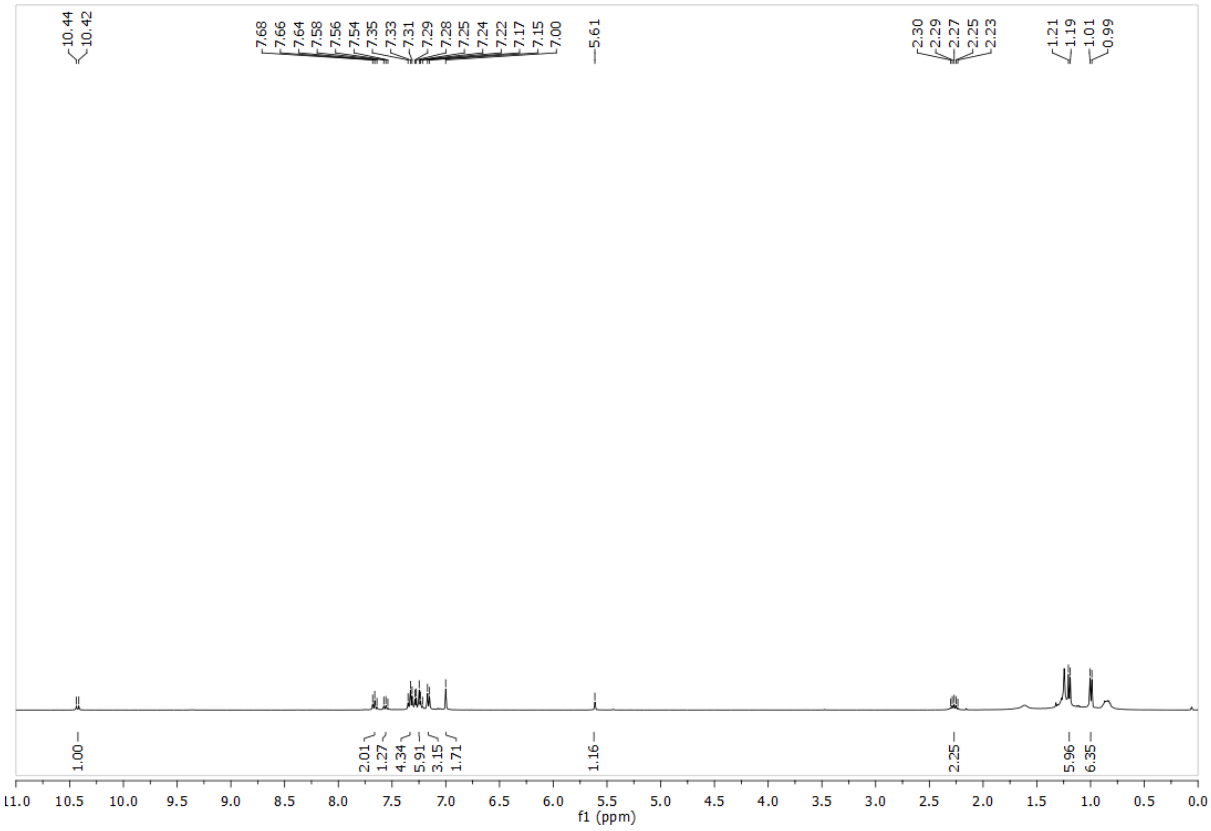


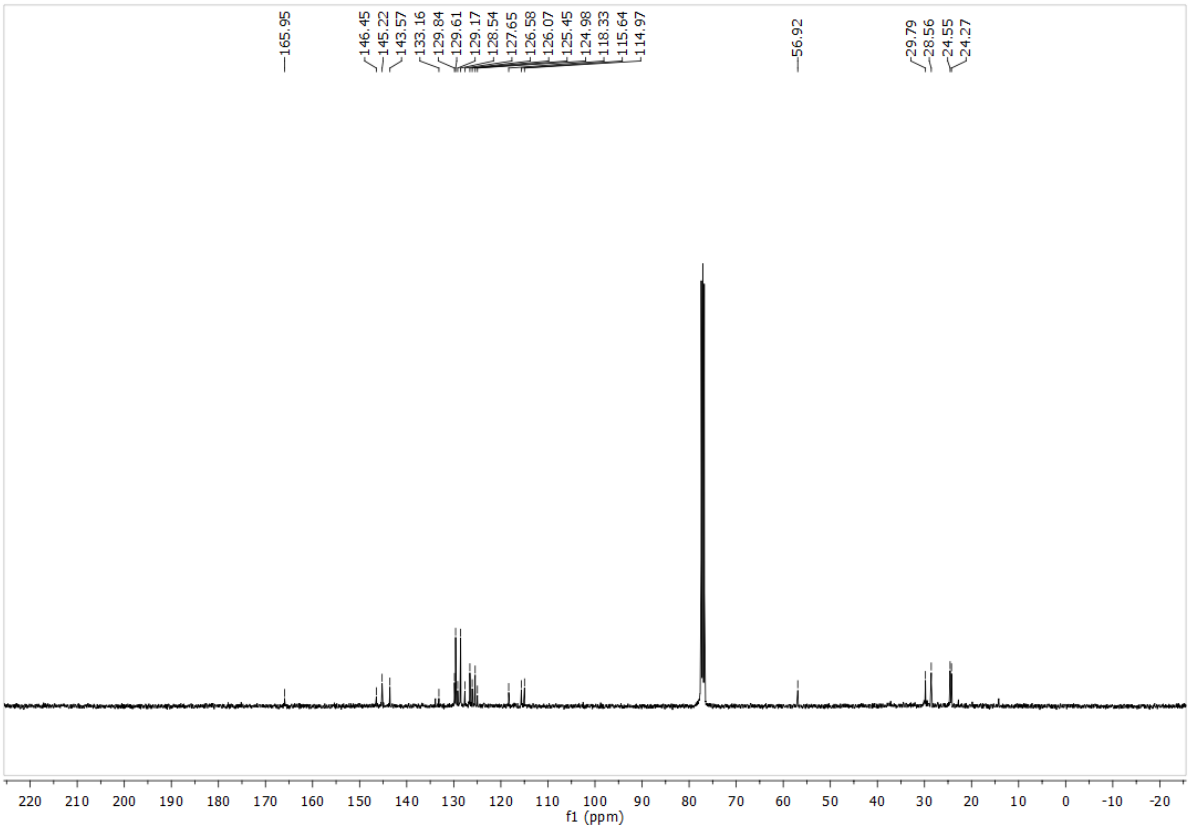
FIG S37 ^{1}H, ^{13}C and HMBC spectra in $CDCl_3$ of AuL6

AuL7:



^{1}H NMR (400 MHz, CHLOROFORM-D) δ 10.43 (d, *J* = 8.4 Hz, 1H), 7.66 (t, *J* = 7.9 Hz, 2H), 7.62 – 7.53 (m, 1H), 7.33 (t, *J* = 7.6 Hz, 4H), 7.29 – 7.21 (m, 6H), 7.16 (d, *J* = 7.6 Hz, 3H), 7.00 (s, 2H), 5.61 (s, 1H), 2.27 (dt, *J* = 13.6, 6.8 Hz, 2H), 1.20 (d, *J* = 6.8 Hz, 6H), 1.00 (d, *J* = 6.8 Hz, 6H).^{13}C NMR (100 MHz, CHLOROFORM-D) δ 165.95, 146.45, 145.22, 143.57, 133.16, 129.84, 129.61, 129.17, 128.54, 127.65, 126.58, 126.07, 125.45, 124.98, 118.33, 115.64, 114.97, 56.92, 29.79, 28.56, 24.55, 24.27.


10.44
10.42
7.68
7.66
7.64
7.58
7.56
7.54
7.35
7.33
7.31
7.29
7.28
7.25
7.24
7.22
7.17
7.15
7.00
5.61
2.30
2.29
2.27
2.25
2.23
1.21
1.19
1.01
0.99
1.00
2.01
1.27
4.34
5.91
3.15
1.71
1.16
2.25
5.96
6.35
f1 (ppm)


165.95
146.45
145.22
143.57
133.16
129.84
129.61
129.17
128.54
127.65
126.58
126.07
125.45
124.98
118.33
115.64
114.97
56.92
29.79
28.56
24.55
24.27
f1 (ppm)

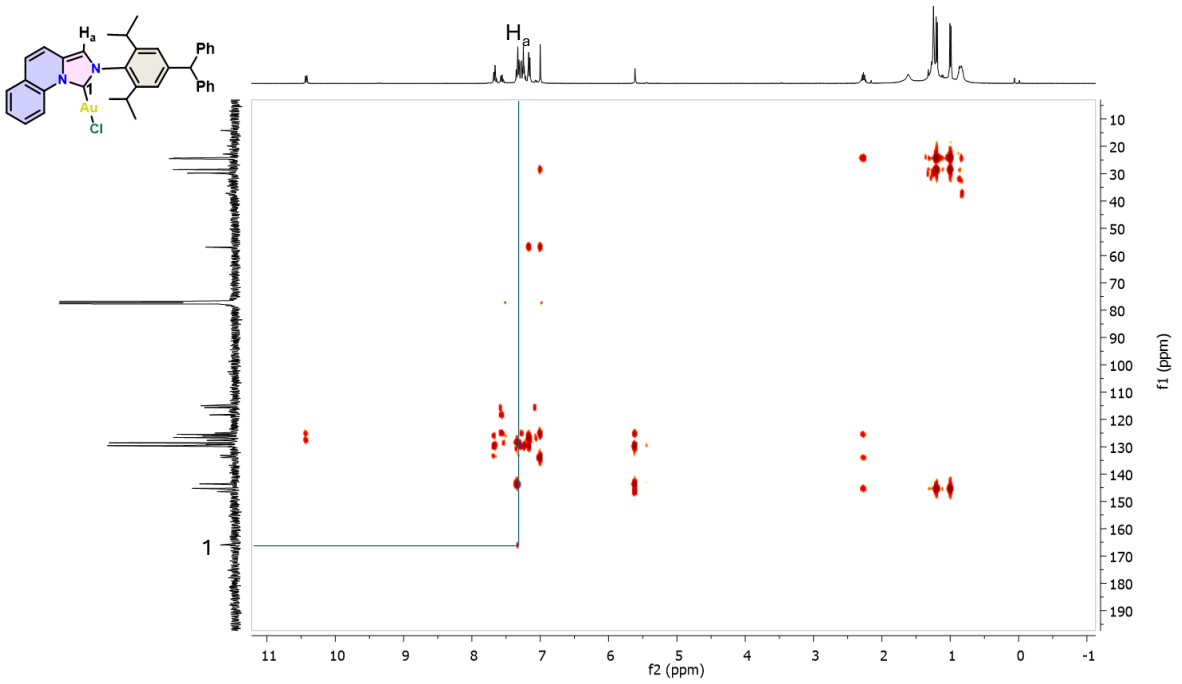


FIG S38. ^{1}H, ^{13}C and HMBC spectra in $CDCl_3$ of AuL7