Synthesis of Ananikov-Type *N*-Heterocyclic Carbene Golden Synthons as Ferroptosis Inducing Anticancer Agents

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Table of Contents

EXPERIMENTAL SECTION

Methods and instruments

Solvents and all other reagents were purchased and used as received without any additional purification, except for K_2CO_3, which was finely grinded using a mortar and pestle, and dried under high vacuum before use. ^{1}H NMR spectra were recorded using Bruker 300 and 400 MHz spectrometers. Chemical shifts (ppm) in ^{1}H and ^{13}C NMR spectra are referenced to the residual solvent peak.^{1}H NMR splitting patterns are abbreviated as follows: broad signal (br), singlet (s), doublet (d), triplet (t), doublet of doublets (dd), doublet of triplets (dt), triplet of triplets (tt), quarter (q), quintet (quint), heptet (hept), multiplet (m). Elemental analyses were carried out using an Elemental CHN "CUBO Micro Vario" analyzer.

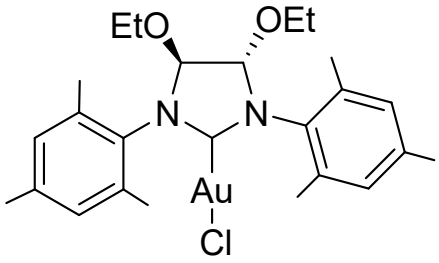
N,N′-diaryl-1,4-diaza-1,3-butadiene precursors (compounds **1** and **2**) and all backbone functionalized azolium salts **3a-f** were synthesized following the procedures described in the literature (see references in the main text of the manuscript).

Computational Methods

All DFT calculations were performed using the Amsterdam Modeling Suite (AMS) software (v. 2020.103).[1,2] The GGA exchange-correlation functional BLYP was used in all geometry optimizations,[3] combined with Grimme's D3 dispersion correction and the Becke-Johnson damping function.[4-9] The Slater-type TZ2P basis set was utilized with the small frozen core approximation.[10] Relativistic corrections were included at the scalar level by means of the Zeroth Order Regular Approximation (ZORA).[11-13] All optimized geometries were assessed via vibrational frequency calculations,[14-16] verifying that transition states display a single imaginary frequency and energy minima display none. The energy of stationary points in solvent was further re-evaluated through single-point calculations with the hybrid PBE0 functional on the all-electron TZ2P basis set.[17,18] Solvation effects were included via a continuum approach in the single-point energies, according to the COnductor-like Screening MOdel (COSMO), with default parameters for ethanol and toluene, depending on the reaction in the main text the calculations are referred to.[19] Therefore, the level of theory of all energy values in the main text is referred to as COSMO-ZORA-PBE0/TZ2P-ae//ZORA-BLYP-D3(BJ)/TZ2P.

Synthesis of NHC-gold-chloride complexes

Synthesis of complex 4a



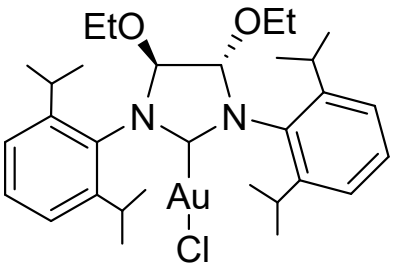
In a 20 mL vial equipped with a stir-bar, 400.1 mg of **3a** (0.93 mmol), 248.4 mg of [Au(DMS)Cl] (0.84 mmol), 351.1 mg of potassium carbonate (2.53 mmol) and 8 mL of acetone were added. The solution was stirred at 60°C for 4 hours. At the end, the solvent was removed under vacuum and dichloromethane was added. Inorganic salts were eliminated by filtration through a small pad of silica. Solvent removal (under vacuum) afforded 483.4 mg of complex **4a** (yield = 91%) as a brownish solid.

^{1}H-NMR (300 MHz, $CDCl_3$, T=298K, ppm): δ 6.93 (m, 4H), 5.02 (s, 2H), 3.43 (m, 4H), 2.44 (s, 6H), 2.31 (s, 6H), 2.26 (s, 6H), 1.13 (t, J = 7.0 Hz, 6H)

^{13}C{^{1}H}-NMR ($CDCl_3$, T=298K, ppm): δ 197.6 (carbene), 138.9, 137.5, 135.1, 133.6, 129.9, 129.5, 98.1, 67.1, 21.1, 18.7, 17.7, 15.3.

Elemental analysis calcd (%) for $C_{25}H_{34}AuClN_2O_2$: C, 47.89; H, 5.47; N, 4.47, found: C, 48.11; H, 5.35; N, 4.41.

Synthesis of complex 4b



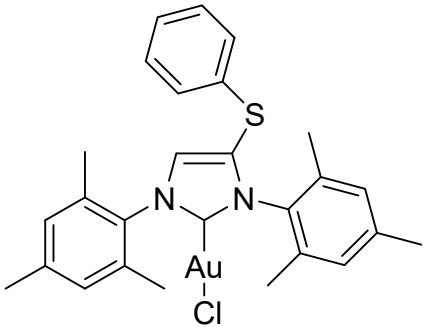
In a 20 mL vial equipped with a stir-bar, 300.4 mg of **3b** (0.58 mmol), 156.4 mg of [Au(DMS)Cl] (0.53 mmol), 219.7 mg of potassium carbonate (1.58 mmol) and 6 mL of acetone were added. The solution was stirred at 60°C for 4 hours. At the end, the solvent was removed under vacuum and dichloromethane was added. Inorganic salts were eliminated by filtration through a small pad of silica. Solvent removal (under vacuum) afforded 377.5 mg of **4b** (yield = 89%) as a white solid.

^{1}H-NMR (300 MHz, $CDCl_3$, T=298K, ppm): δ 7.44 (t, *J* = 7.7 Hz, 2H), 7.25 (m, 4H), 5.00 (s, 2H), 3.47 (q, *J* = 7.0 Hz, 4H), 3.37 (m, 2H), 3.00 (m, 2H), 1.45 (d, *J* = 6.9 Hz, 6H), 1.37 (dd, *J* = 6.8, 5.1 Hz, 12H), 1.31 (d, *J* = 6.8 Hz, 6H), 1.18 (t, *J* = 7.0 Hz, 6H).

^{13}C{^{1}H}-NMR ($CDCl_3$, T=298K, ppm): δ 198.3 (carbene), 148.6, 146.1, 132.6, 130.1, 124.8, 124.2, 99.2, 66.6, 28.6, 28.5, 25.7, 25.3, 23.9, 23.7, 15.1.

Elemental analysis calcd (%) for $C_{31}H_{46}AuClN_2O_2$: C, 52.36; H, 6.52; N, 3.94, found: C, 52.01; H, 5.43; N, 4.12.

Synthesis of complex 4c



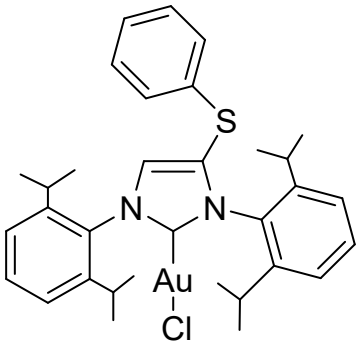
In a 20 mL vial equipped with a stir-bar, 402.1 mg of **3c** (0.89 mmol), 239.2 mg of [Au(DMS)Cl] (0.81 mmol), 336.8 mg of potassium carbonate (2.43 mmol) and 8 mL of acetone were added. The solution was stirred at 60°C for 4 hours. At the end, the solvent was removed under vacuum and dichloromethane was added. Inorganic salts were eliminated by filtration through a small pad of silica. Solvent removal (under vacuum) afforded 575.5 mg of **4c** (yield >99%) as a white solid.

^{1}H-NMR (300 MHz, $CDCl_3$, T=298K, ppm): δ 7.31 (m, 1H), 7.24 (m, 2H), 7.11 (m, 2H), 7.01 (m, 2H), 6.90 (m, 2H), 2.36 (s, 6H), 2.13 (s, 6H), 1.78 (s, 6H)

^{13}C{^{1}H}-NMR ($CDCl_3$, T=298K, ppm): δ 175.6 (carbene), 139.9, 139.8, 135.4, 134.5, 134.5, 132.5, 129.5, 129.3, 129.3, 128.9, 126.2, 21.2, 21.1, 17.8, 17.7.

Elemental analysis calcd (%) for $C_{27}H_{28}AuClN_2S$: C, 50.28; H, 4.38; N, 4.34, found: C, 50.59; H, 4.17; N, 4.21.

Synthesis of complex 4d



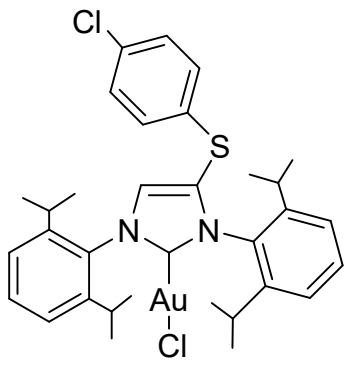
In a 20 mL vial equipped with a stir-bar, 400.7 mg of **3d** (0.75 mmol), 201.1 mg of [Au(DMS)Cl] (0.68 mmol), 282.6 mg of potassium carbonate (2.1 mmol) and 8 mL of acetone were added. The solution was stirred at 60°C for 4 hours. At the end, the solvent was removed under vacuum and dichloromethane was added. Inorganic salts were eliminated by filtration through a small pad of silica. Solvent removal (under vacuum) afforded 449.5 mg of **4d** (yield = 90%) as a white solid.

^{1}H-NMR (300 MHz, $CDCl_3$, T=298K, ppm): δ 7.52 (m, 2H), 7.33 (m, 3H), 7.26 (m, 6H), 7.15 (s, 1H), 2.63 (hept, *J* = 6.9 Hz, 2H), 2.39 (hept, *J* = 6.9 Hz, 2H), 1.37 (dd, *J* = 6.9, 5.0 Hz, 12H), 1.26 (d, *J* = 6.9 Hz, 6H), 1.04 (d, *J* = 6.8 Hz, 6H).

^{13}C{^{1}H}-NMR ($CDCl_3$, T=298K, ppm): δ 177.0 (carbene), 146.1, 145.4, 131.0, 130.9, 129.8, 129.7, 128.4, 126.7, 124.3, 124.2, 29.1, 28.9, 25.2, 24.4, 24.1, 22.9.

Elemental analysis calcd (%) for $C_{33}H_{40}AuClN_2S$: C, 54.36; H, 5.53; N, 3.84, found: C, 54.60; H, 5.31; N, 3.69.

Synthesis of complex 4e



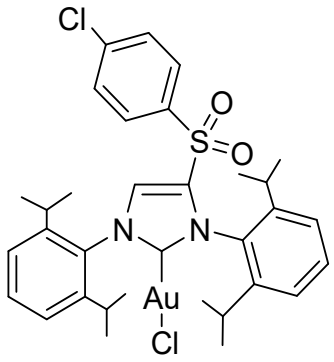
In a 20 mL vial equipped with a stir-bar, 402.1 mg of **3e** (0.71 mmol), 189.1 mg of [Au(DMS)Cl] (0.64 mmol), 266.5 mg of potassium carbonate (1.9 mmol) and 8 mL of acetone were added. The solution was stirred at 60°C for 4 hours. At the end, the solvent was removed under vacuum and dichloromethane was added. Inorganic salts were eliminated by filtration through a small pad of silica. Solvent removal (under vacuum) afforded 487.2 mg of **4e** (yield > 99%) as a white solid.

^{1}H-NMR (300 MHz, $CDCl_3$, T=298K, ppm): δ 7.53 (m, 2H), 7.31 (m, 3H), 7.27 (m, 3H), 7.17 (m, 3H), 2.61 (hept, *J* = 6.9 Hz, 2H), 2.35 (hept, *J* = 6.8 Hz, 2H), 1.37 (dd, *J* = 6.9, 4.5 Hz, 12H), 1.26 (d, *J* = 6.9 Hz, 6H), 1.05 (d, *J* = 6.8 Hz, 6H).

^{13}C{^{1}H}-NMR ($CDCl_3$, T=298K, ppm): δ 177.5 (carbene), 146.1, 145.3, 131.1, 131.1, 131.0, 129.9, 127.0, 124.4, 124.3, 29.1, 28.9, 25.2, 24.4, 24.1, 22.9.

Elemental analysis calcd (%) for $C_{33}H_{39}AuCl_2N_2S$: C, 51.84; H, 5.27; N, 3.66, found: C, 51.57; H, 5.39; N, 3.78.

Synthesis of complex 4f



In a 20 mL vial equipped with a stir-bar, 399.7 mg of **3f** (0.66 mmol), 178.7 mg of [Au(DMS)Cl] (0.61 mmol), 251.9 mg of potassium carbonate (1.8 mmol) and 8 mL of acetone were added. The solution was stirred at 60°C for 4 hours. At the end, the solvent was removed under vacuum and dichloromethane was added. Inorganic salts were eliminated by filtration through a small pad of silica. Solvent removal (under vacuum) afforded 347.4 mg of **4f** (yield = 72%) as a white solid.

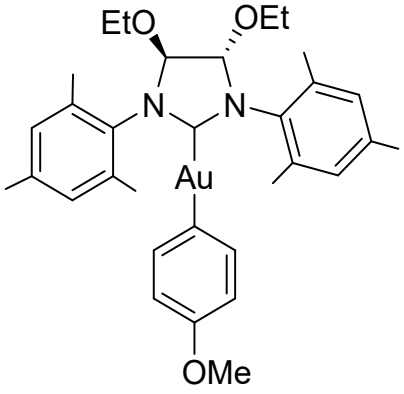
^{1}H NMR (300 MHz, $CDCl_3$, T=298K, ppm): δ 7.53 (m, 2H), 7.31 (m, 3H), 7.27 (m, 3H), 7.18 (m, 3H), 2.61 (hept, *J* = 6.8 Hz, 2H), 2.35 (hept, *J* = 6.8 Hz, 2H), 1.37 (dd, *J* = 6.9, 4.5 Hz, 12H), 1.26 (d, *J* = 6.9 Hz, 6H), 1.04 (d, *J* = 6.9 Hz, 6H).

^{13}C{^{1}H}-NMR ($CDCl_3$, T=298K, ppm): δ 177.4, 146.1, 145.3, 131.4, 131.1, 131.1, 131.0, 129.9, 127.6, 127.0, 124.4, 124.3, 29.1, 28.9, 25.2, 24.4, 24.1, 22.9.

Elemental analysis calcd (%) for $C_{33}H_{39}AuCl_2N_2O_2S$: : C, 49.76; H, 5.06; N, 3.52, found: C, 50.02; H, 4.91; N, 3.33.

Synthesis of NHC-gold-aryl complexes

Synthesis of complex 5a



In a 20 mL vial equipped with a stir-bar, 100.6 mg of **4a** (0.16 mmol), 27.3 mg of 4-methoxyphenylboronic acid (0.17 mmol), 66.4 mg of potassium carbonate (0.48 mmol) and 6.5 mL of ethanol were added. The solution was stirred at 40°C for 24 hours. Afterwards, the solvent was removed and dichloromethane was added. Inorganic salts were eliminated by filtration on PTFE microfilter and the filtrate was concentrated and precipitated with pentane.

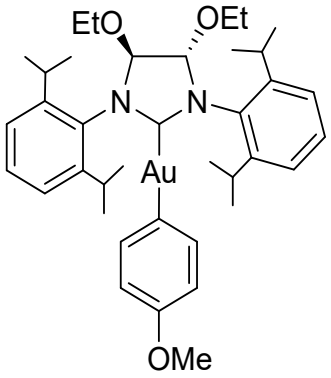
This process afforded 81.3 mg of **5a** (yield = 73%) as a white solid.

^{1}H-NMR (300 MHz, $CDCl_3$, T=298K, ppm) δ 6.95 (m, 6H), 6.65 (m, 2H), 5.01 (s, 2H), 3.68 (s, 3H), 3.45 (m, 4H), 2.53 (s, 6H), 2.31 (d, J = 10.7 Hz, 12H), 1.14 (t, J = 7.0 Hz, 6H).

^{13}C{^{1}H}-NMR ($CDCl_3$, T=298K, ppm): δ 219.0 (carbene), 140.8, 138.2, 137.8, 135.3, 134.4, 129.5, 129.4, 129.3, 129.2, 112.6, 98.2, 77.2, 67.3, 66.7, 54.9, 21.1, 19.0, 17.9, 15.4, 15.2.

Elemental analysis calcd (%) for $C_{32}H_{41}AuN_2O_3$: C, 55.01; H, 5.92; N, 4.01, found: C, 55.29; H, 5.82; N, 3.89.

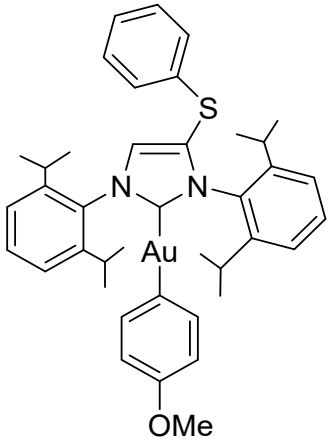
Synthesis of complex 5b



In a 20 mL vial equipped with a stir-bar, 100.4 mg of **4b** (0.14 mmol), 24.1 mg of 4-methoxyphenylboronic acid (0.15 mmol), 64.6 mg of potassium carbonate (0.46 mmol) and 6.5 mL of ethanol were added. The solution was stirred at 40°C for 24 hours. Afterwards, the solvent was removed and dichloromethane was added. Inorganic salts were eliminated by filtration on PTFE microfilter and the filtrate was concentrated and precipitated with pentane.
This process afforded 88.1 mg of **5b** (yield = 79%) as a white solid.

^{1}H NMR (300 MHz, $CDCl_3$, T=298K, ppm): δ 7.41 (m, 2H), 7.27 – 7.15 (m, 4H), 6.94 (m, 2H), 6.64 (m, 2H), 4.98 (d, *J* = 1.2 Hz, 2H), 3.66 (d, *J* = 1.2 Hz, 2H), 3.55 (m, 4H), 3.06 (m, 2H),1,61 (s, 3H) 1.54 (d, *J* = 6.8 Hz, 6H), 1.36 (m, 18H), 1.18 (m, 6H).
^{13}C{^{1}H}-NMR ($CDCl_3$, T=298K, ppm): δ 219.4 (carbene), 148.8, 146.3, 140.7, 133.3, 129.5, 124.6, 124.3, 123.9, 112.5, 99.7, 99.1, 77.2, 66.2, 54.9, 28.5, 28.4, 25.7, 25.6, 25.2, 23.9, 23.8, 23.6, 15.1.
Elemental analysis calcd (%) for $C_{38}H_{53}AuN_2O_3$: C, 58.30; H, 6.82; N, 3.58, found: C, 58.56; H, 6.71; N, 3.42.

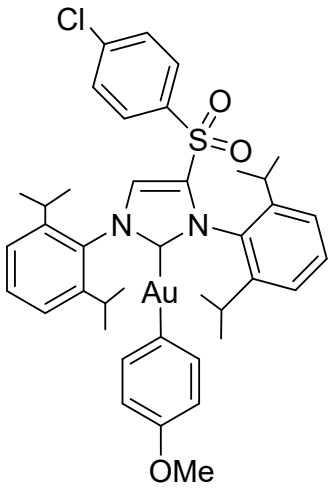
Synthesis of complex 5d



In a 20 mL vial equipped with a stir-bar, 100.7 mg of **4d** (0.14 mmol), 23.6 mg of 4-methoxyphenylboronic acid (0.15 mmol), 57.6 mg of potassium carbonate (0.41 mmol) and 6.5 mL of ethanol were added. The solution was stirred at 40°C for 24 hours. Afterwards, the solvent was removed and dichloromethane was added. Inorganic salts were eliminated by filtration on PTFE microfilter and the filtrate was concentrated and precipitated with pentane.
This process afforded 88.6 mg of **5d** (yield = 83%) as a white solid.

^{1}H-NMR (300 MHz, $CDCl_3$, T=298K, ppm): δ 7.48 (m, 2H), 7.30 (d, *J* = 8.0 Hz, 4H), 7.25 (m, 7H), 7.01 (m, 2H), 6.65 (m, 2H), 3.68 (s, 3H), 2.76 (p, *J* = 6.9 Hz, 2H), 2.45 (p, *J* = 6.9 Hz, 2H), 1.43 (dd, *J* = 6.9, 4.9 Hz, 12H), 1.30 (d, *J* = 6.9 Hz, 6H), 1.01 (d, *J* = 6.9 Hz, 6H).
^{13}C{^{1}H}-NMR ($CDCl_3$, T=298K, ppm): δ 199.2 (carbene), 159.9, 156.7, 146.3, 145.6, 140.7, 134.5, 132.6, 132.1, 130.3, 130.3, 129.5, 129.1, 127.8, 127.7, 126.6, 124.0, 123.8, 112.6, 77.4, 77.2, 77.0, 76.6, 54.9, 29.1, 28.9, 25.2, 24.4, 24.0, 22.8.
Elemental analysis calcd (%) for $C_{40}H_{47}AuN_2OS$: C, 59.99; H, 5.92; N, 3.50, found: C, 60.34; H, 5.79; N, 3.36.

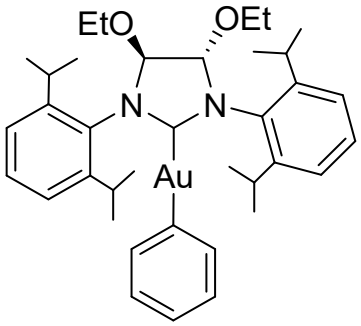
Synthesis of complex 5f



In a 20 mL vial equipped with a stir-bar, 100.3 mg of **4f** (0.12 mmol), 20.8 mg of 4-methoxyphenylboronic acid (0.14 mmol), 53.3 mg of potassium carbonate (0.37 mmol) and 6.5 mL of ethanol were added. The solution was stirred at 40°C for 24 hours. Afterwards, the solvent was removed and dichloromethane was added. Inorganic salts were eliminated by filtration on PTFE microfilter and the filtrate was concentrated and precipitated with pentane.
This process afforded 115.1 mg of **5f** (yield = 83%) as a white solid.

^{1}H NMR (300 MHz, $CDCl_3$, T=298K, ppm): δ 7.48 (m, 1H), 7.31 (d, *J* = 3.9 Hz, 2H), 7.20 (m, 8H), 6.99 (d, *J* = 8.4 Hz, 2H), 6.65 (m, 2H), 3.67 (s, 3H), 2.70 (m, 2H), 2.38 (dp, *J* = 13.8, 6.8 Hz, 2H), 1.42 (dd, *J* = 6.8, 3.8 Hz, 12H), 1.28 – 1.25 (m, 6H), 1.02 (dd, *J* = 6.9, 4.3 Hz, 6H).
^{13}C{^{1}H}-NMR ($CDCl_3$, T=298K, ppm): δ 199.7 (carbene), 159.7, 156.8, 146.2, 146.2, 145.5, 145.4, 140.6, 134.3, 132.0, 131.1, 130.8, 130.7, 130.4, 130.4, 129.9, 129.8, 129.6, 128.0, 127.3, 124.2, 124.2, 124.0, 123.9, 112.6, 77.4, 77.2, 77.0, 76.6, 54.9, 29.1, 29.1, 28.9, 25.2, 25.1, 24.4, 24.2, 24.1, 24.0, 22.9, 22.8, 18.4.
Elemental analysis calcd (%) for $C_{40}H_{46}AuClN_2O_3S$: C, 55.40; H, 5.35; N, 3.23, found: C, 55.09; H, 5.44; N, 3.31.

Synthesis of complex 6b



In a 20 mL vial equipped with a stir-bar, 201.3 mg of **4b** (0.28 mmol), 37.6 mg of phenylboronic acid (0.31 mmol), 116.8 mg of potassium carbonate (0.84 mmol) and 13 mL of ethanol were added. The solution was stirred at 40°C for 24 hours. Afterwards, the solvent was removed and dichloromethane was added. Inorganic salts were eliminated by filtration on PTFE microfilter and the filtrate was concentrated and precipitated with pentane.

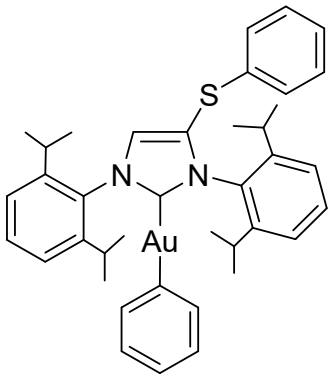
This process afforded 202.6 mg of **6b** (yield = 96%) as a white solid.

^{1}H-NMR (300 MHz, $CDCl_3$, T=298K, ppm): δ 7.38-7.36 (m, 1H), 7.34 – 7.29 (m, 2H), 7.22-7.17 (m, 6H), 7.13 (dd, *J* = 7.5, 1.8 Hz, 1H), 4.99 (s, 2H), 3.51-3.43 (m, 4H), 3.11-3.00 (m, 2H), 1.55 (d, *J* = 6.9 Hz, 4H), 1.25-1.20 (m, 18H) 1.54 (d, *J* = 6.8 Hz, 6H), 1.36 (m, 18H), 0.77 (t, *J* = 7.0 Hz, 3H).

^{13}C{^{1}H}-NMR ($CDCl_3$, T=298K, ppm): δ 169.7, 148.8, 146.3, 140.4, 133.2, 129.5, 126.5, 124.3, 124.1, 123.9, 99.7, 77.3, 77.0, 76.7, 66.3, 28.5, 28.4, 25.6, 25.2, 23.9, 23.6, 15.1.

Elemental analysis calcd (%) for $C_{37}H_{51}AuN_2O_2$: C, 59.03; H, 6.83; N, 3.72, found: C, 58.86; H, 6.97; N, 3.64.

Synthesis of complex 6d



In a 20 mL vial equipped with a stir-bar, 200.9 mg of **4d** (0.27 mmol), 37.2 mg of phenylboronic acid (0.30 mmol), 113.7 mg of potassium carbonate (0.82 mmol) and 13 mL of ethanol were added. The solution was stirred at 40°C for 24 hours. Afterwards, the solvent was removed and dichloromethane was added. Inorganic salts were eliminated by filtration on PTFE microfilter and the filtrate was concentrated and precipitated with pentane.

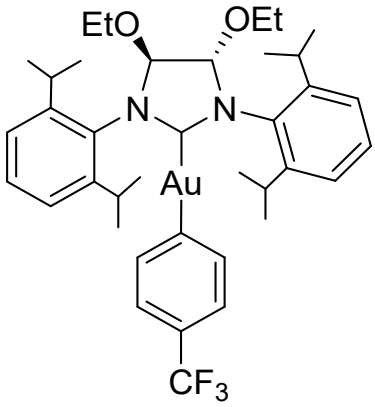
This process afforded 187.9 mg of **6d** (yield = 89%) as a white solid.

^{1}H-NMR (300 MHz, $CDCl_3$, T=298K, ppm): δ 7.47 (m, 2H), 7.30 (m, 2H), 7.26 (m, 6H), 7.3 (m, 4H), 6.82 (m, 1H), 2.75 (p, *J* = 6.9 Hz, 2H), 2.44 (p, *J* = 6.9 Hz, 2H), 1.42 (dd, *J* = 6.8, 4.9 Hz, 12H), 1.29 (d, *J* = 6.9 Hz, 6H), 1.01 (d, *J* = 6.9 Hz, 6H).

^{13}C{^{1}H}-NMR ($CDCl_3$, T=298K, ppm): δ 199.2 (carbene), 169.1, 146.3, 145.6, 140.5, 134.5, 132.6, 132.1, 130.3, 130.3, 129.5, 129.1, 127.8, 127.6, 126.8, 126.6, 124.2, 124.0, 123.8, 77.3, 77.0, 76.7, 29.1, 28.9, 25.1, 24.4, 24.0, 22.8.

Elemental analysis calcd (%) for $C_{39}H_{45}AuN_2S$: C, 60.77; H, 5.88; N, 3.63, found: C, 61.03; H, 5.70; N, 3.54.

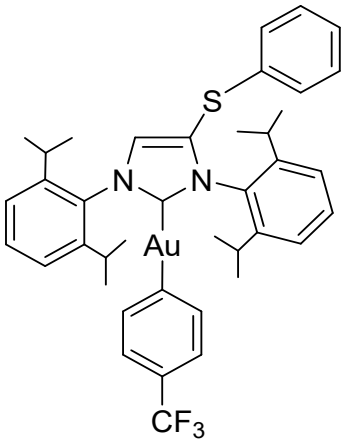
Synthesis of complex 7b



In a 20 mL vial equipped with a stir-bar, 161.8 mg of **4b** (0.22 mmol), 47.8 mg of 4-trifluoromethylphenylboronic acid (0.25 mmol), 93.3 mg of potassium carbonate (0.67 mmol) and 10 mL of ethanol were added. The solution was stirred at 40°C for 24 hours. Afterwards, the solvent was removed and dichloromethane was added. Inorganic salts were eliminated by filtration on PTFE microfilter and the filtrate was concentrated and precipitated with pentane.
This process afforded 186.2 mg of **7b** (yield > 99%) as a white solid.

^{1}H-NMR (300 MHz, $CDCl_3$, T=298K, ppm): δ 7.41 (t, *J* = 7.7 Hz, 2H), 7.21 (m, 5H), 7.07 (m, 2H), 5.01 (s, 2H), 3.49 (q, *J* = 7.0 Hz, 6H), 3.07 (p, *J* = 6.8 Hz, 2H), 1.53 (d, *J* = 6.9 Hz, 6H), 1.36 (m, 18H), 1.19 (t, *J* = 7.0 Hz, 6H).
^{13}C{^{1}H}-NMR ($CDCl_3$, T=298K, ppm): δ 218.4 (carbene), 175.0, 148.8, 146.3, 140.1, 133.1, 129.7, 126.2, 126.0, 125.7, 124.4, 124.0, 122.5, 122.4, 122.4, 122.4, 99.7, 77.3, 77.0, 76.7, 66.4, 29.7, 28.5, 28.4, 25.6, 25.2, 23.9, 23.6, 15.1.
Elemental analysis calcd (%) for $C_{38}H_{50}AuF_3N_2O_2$: C, 55.61; H, 6.14; N, 3.41, found: C, 55.89; H, 6.03; N, 3.31.

Synthesis of complex 7d

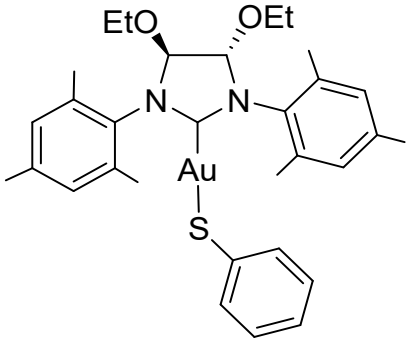


In a 20 mL vial equipped with a stir-bar, 155.2 mg of **4d** (0.21 mmol), 44.6 mg of 4-trifluoromethylphenylboronic acid (0.23 mmol), 88.1 mg of potassium carbonate (0.64 mmol) and 12 mL of ethanol were added. The solution was stirred at 40°C for 24 hours. Afterwards, the solvent was removed and dichloromethane was added. Inorganic salts were eliminated by filtration on PTFE microfilter and the filtrate was concentrated and precipitated with pentane.
This process afforded 117 mg of **7d** (yield = 65%) as a white solid.

^{1}H-NMR (300 MHz, $CDCl_3$, T=298K, ppm): δ 7.50 (t, *J* = 7.7 Hz, 2H), 7.31 (d, *J* = 7.8 Hz, 4H), 7.25 (m, 9H), 7.14 (m, 2H), 2.73 (p, *J* = 6.9 Hz, 2H), 2.44 (p, *J* = 6.8 Hz, 2H), 1.41 (dd, *J* = 6.8, 5.3 Hz, 12H), 1.30 (d, *J* = 6.9 Hz, 6H), 1.02 (d, *J* = 6.8 Hz, 6H).
^{13}C{^{1}H}-NMR ($CDCl_3$, T=298K, ppm): δ 198.0 (carbene), 174.4, 146.3, 145.6, 140.2, 134.3, 132.4, 132.0, 130.5, 130.5, 129.6, 129.3, 127.9, 127.6, 127.2, 126.3, 126.1, 125.8, 124.1, 123.9, 123.6, 122.6, 122.6, 122.5, 122.5, 77.3, 77.1, 76.7, 29.1, 28.9, 25.2, 24.4, 24.0, 22.9.
Elemental analysis calcd (%) for $C_{40}H_{44}AuF_3N_2S$: C, 57.28; H, 5.29; N, 3.34, found: C, 56.96; H, 5.40; N, 3.43.

Synthesis of NHC-gold-thiolate complexes

Synthesis of complex 8a



In a 20 mL vial equipped with a stir-bar, 121 mg of **4a** (0.19 mmol), 23.6 mg of thiophenol (0.21 mmol), 82.9 mg of potassium carbonate (0.57 mmol) and 6 mL of ethanol were added. The solution was stirred at room temperature for 3 hours. Afterwards, the solvent was removed and dichloromethane was added. Inorganic salts were eliminated by filtration on PTFE microfilter and the filtrate was concentrated and precipitated with pentane.

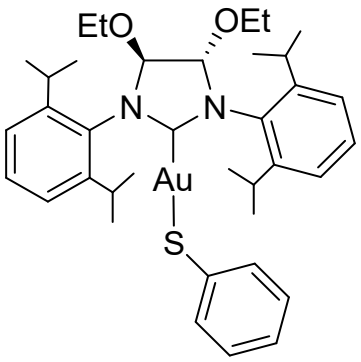
This process afforded 133.6 mg of **8a** (yield >99%) as a white solid.

^{1}H-NMR (300 MHz, $CDCl_3$, T=298K, ppm): δ 6.71-7.05 (m, 9H), 5.06 (s, 2H), 3.47 (p, J = 8.1, 7.2 Hz, 4H), 2.48 (s, 6H), 2.36 (s, 6H), 2.31 (s, 6H), 1.15 (t, J = 7.0 Hz, 6H).

^{13}C{^{1}H}-NMR ($CDCl_3$, T=298K, ppm): δ 207.8 (carbene), 148.9, 146.6, 143.3, 132.8, 131.5, 130.0, 127.1, 124.7, 124.2, 121.7, 99.7, 77.3, 77.0, 76.7, 66.7, 28.6, 28.5, 25.6, 25.2, 24.0, 23.9, 15.1.

Elemental analysis calcd (%) for $C_{31}H_{39}AuN_2O_2S$: C, 53.14; H, 5.61; N, 4.00, found: C, 52.87; H, 5.77; N, 4.09.

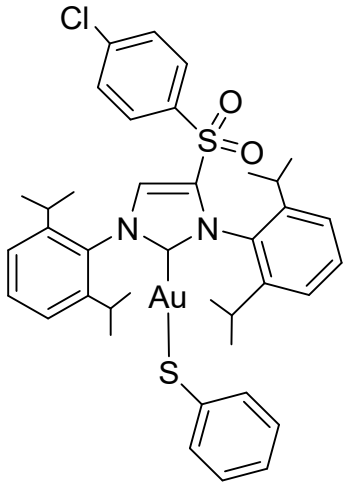
Synthesis of complex 8b



In a 20 mL vial equipped with a stir-bar, 119.8 mg of **4b** (0.16 mmol), 20.8 mg of thiophenol (0.18 mmol), 71.4 mg of potassium carbonate (0.50 mmol) and 6 mL of ethanol were added. The solution was stirred at room temperature for 3 hours. Afterwards, the solvent was removed and dichloromethane was added. Inorganic salts were eliminated by filtration on PTFE microfilter and the filtrate was concentrated and precipitated with pentane.
This process afforded 131.8 mg of **8b** (yield = 98%) as a white solid.

^{1}H-NMR (300 MHz, $CDCl_3$, T=298K, ppm): δ 7.45-7.54 (m, 2H), 7.23-7.34 (m, 4H), 6.65-6.78 (m, 4H), 5.06 (s, 2H), 3.37-3.59 (m, 6H), 3.07 (p, *J* = 6.8 Hz, 2H), 1.28-1.46 (m, 24H), 1.19 (t, *J* = 7.0, 6H).
^{13}C{^{1}H}-NMR ($CDCl_3$, T=298K, ppm): δ 207.8 (carbene), 148.9, 146.6, 143.3, 132.8, 131.5, 130.0, 127.1, 124.7, 124.2, 121.7, 99.7, 77.3, 77.2, 77.0, 76.7, 66.7, 28.6, 28.5, 25.6, 25.2, 24.0, 23.9, 15.1.
Elemental analysis calcd (%) for $C_{37}H_{51}AuN_2O_2S$: C, 56.62; H, 6.55; N, 3.57, found: C, 56.97; H, 6.32; N, 3.45.

Synthesis of complex 8f



In a 20 mL vial equipped with a stir-bar, 119.9 mg of **4f** (0.15 mmol), 18.5 mg of thiophenol (0.16 mmol), 64.1 mg of potassium carbonate (0.45 mmol) and 6 mL of ethanol were added. The solution was stirred at room temperature for 3 hours. Afterwards, the solvent was removed and dichloromethane was added. Inorganic salts were eliminated by filtration on PTFE microfilter and the filtrate was concentrated and precipitated with pentane.

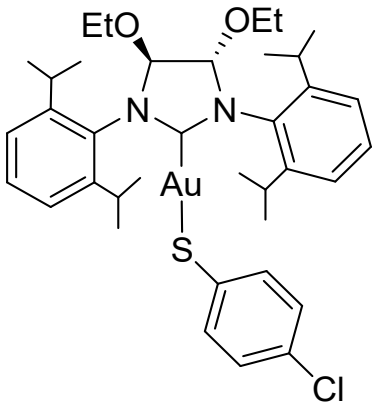
This process afforded 129 mg of **8f** (yield = 98%) as a white solid.

^{1}H-NMR (300 MHz, $CDCl_3$, T=298K, ppm): δ 7.63-7.48 (m, 3H), 7.37-7.29 (m, 7H), 7.19 (d, *J* = 8.6 Hz, 1H), 6.85-6.70 (m, 5H), 2.68 (p, *J* = 6.9 Hz, 2H), 2.40 (p, *J* = 6.8 Hz, 2H), 1.36 (dd, *J* = 6.9, 4.4 Hz, 12H), 1.28 (d, *J* = 6.8 Hz, 6H), 1.04 (d, *J* = 6.8 Hz, 6H).

^{13}C{^{1}H}-NMR ($CDCl_3$, T=298K, ppm): δ 188.87 (carbene), 146.39, 145.66, 143.42, 134.49, 133.97, 131.61, 130.90, 130.84, 130.77, 130.45, 129.86, 129.09, 127.47, 127.39, 127.25, 127.17, 126.96, 124.35, 124.29, 121.87, 77.47, 77.25, 77.05, 76.62, 29.74, 29.23, 29.01, 25.19, 24.34, 24.22, 23.00.

Elemental analysis calcd (%) for $C_{39}H_{44}AuClN_2O_2S_2$: C, 53.88; H, 5.10; N, 3.22, found: C, 54.04; H, 4.97; N, 3.11.

Synthesis of complex 9b



In a 20 mL vial equipped with a stir-bar, 121.6 mg of **4b** (0.17 mmol), 31 mg of thiophenol(-4-Cl) (0.21 mmol), 69.9 mg of potassium carbonate (0.51 mmol) and 6 mL of ethanol were added. The solution was stirred at room temperature for 3 hours. Afterwards, the solvent was removed and dichloromethane was added. Inorganic salts were eliminated by filtration on PTFE microfilter and the filtrate was concentrated and precipitated with pentane.

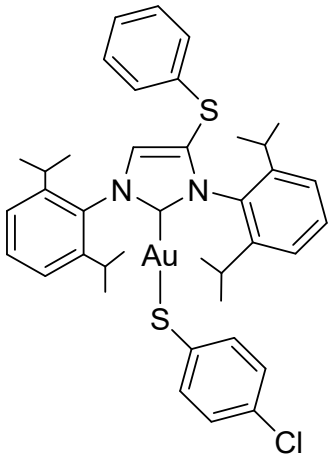
This process afforded 139.4 mg of **9b** (yield > 99%) as a white solid.

^{1}H-NMR (300 MHz, $CDCl_3$, T=298K, ppm): δ 7.50 (t, *J* = 7.7 Hz, 2H), 7.31 (d, *J* = 1.5 Hz, 2H), 7.27 (d, *J* = 5.4 Hz, 2H), 6.69 (d, *J* = 8.5 Hz, 2H), 6.57 (d, *J* = 8.5 Hz, 2H), 5.06 (s, 2H), 3.48 (dq, *J* = 17.6, 6.9 Hz, 6H), 3.05 (p, *J* = 6.9 Hz, 2H), 1.39 (m, 18H), 1.31 (d, *J* = 6.7 Hz, 6H), 1.19 (t, *J* = 7.0 Hz, 6H).

^{13}C{^{1}H}-NMR ($CDCl_3$, T=298K, ppm): δ 199.2 (carbene), 199.2, 159.9, 156.7, 146.3, 145.6, 140.7, 134.5, 132.6, 132.1, 130.3, 130.3, 129.5, 129.1, 127.8, 127.7, 126.6, 126.6, 124.0, 123.8, 112.6, 77.4, 77.0, 76.6, 29.1, 28.9, 25.2, 24.4, 24.0, 22.8.

Elemental analysis calcd (%) for $C_{37}H_{50}AuClN_2O_2S$: C, 54.24; H, 6.15; N, 3.42, found: C, 54.45; H, 6.02; N, 3.34.

Synthesis of complex 9d

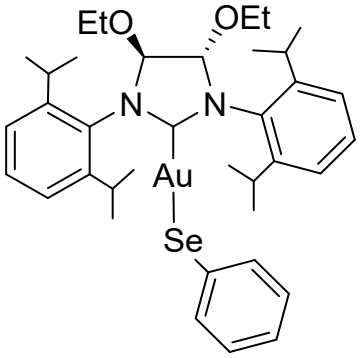


In a 20 mL vial equipped with a stir-bar, 120.4 mg of **4d** (0.16 mmol), 26.6 mg of thiophenol(-4-Cl) (0.18 mmol), 68.7 mg of potassium carbonate (0.49 mmol) and 6 mL of ethanol were added. The solution was stirred at room temperature for 3 hours. Afterwards, the solvent was removed and dichloromethane was added. Inorganic salts were eliminated by filtration on PTFE microfilter and the filtrate was concentrated and precipitated with pentane.
This process afforded 118.4 mg of **9d** (yield = 88%) as a white solid.

^{1}H-NMR (300 MHz, $CDCl_3$, T=298K, ppm): δ 7.58 (td, *J* = 7.8, 4.7 Hz, 2H), 7.33 (m, 7H), 7.26 (d, *J* = 12.9 Hz, 3H), 2.69 (p, *J* = 6.9 Hz, 2H), 2.42 (p, *J* = 6.8 Hz, 2H), 1.35 (dd, *J* = 6.9, 5.6 Hz, 12H), 1.28 (d, *J* = 6.9 Hz, 6H), 1.04 (d, *J* = 6.8 Hz, 6H).
^{13}C{^{1}H}-NMR ($CDCl_3$, T=298K, ppm): δ 187.9 (carbene), 146.4, 145.7, 142.3, 134.1, 132.7, 131.8, 131.7, 130.8, 130.8, 129.7, 129.6, 128.3, 127.9, 127.4, 127.1, 124.3, 124.2, 77.5, 77.3, 77.1, 76.6, 29.2, 28.9, 25.2, 24.4, 24.2, 23.1.
Elemental analysis calcd (%) for $C_{39}H_{44}AuClN_2S_2$: C, 55.94; H, 5.30; N, 3.35, found: C, 56.21; H, 5.12; N, 3.27.

Synthesis of NHC-gold-selenolate complexes

Synthesis of complex 10b



In a 10 mL vial equipped with a stir-bar, 61.1 mg of **6b** (0.07 mmol), 19.4 mg of elemental selenium (0.24 mmol), and 4 mL of anhydrous toluene were added under argon atmosphere. The solution was stirred at 110°C for 24 hours. The solution is yellow with a black precipitate in it. During the reaction the solution change to orange. Afterwards, the solvent was removed and dichloromethane was added. Elemental selenium was eliminated by filtration on PTFE microfilter and the filtrate was concentrated and precipitated with pentane.

This process afforded 58.5 mg of **10b** (yield = 88%) as an orange solid.

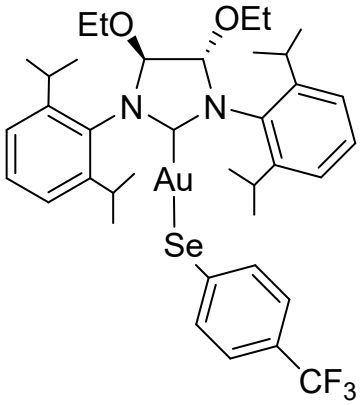
^{1}H-NMR (400 MHz, $CDCl_3$, T=298K, ppm): δ 7.46 (t, *J* = 7.7 Hz, 2H), 7.27 (d, *J* = 1.5 Hz, 1H), 7.24 (m, 3H), 6.82 (m, 2H), 6.70 (dd, *J* = 8.6, 6.6 Hz, 2H), 5.03 (s, 2H), 3.51 – 3.37 (m, 6H), 3.05 (p, *J* = 6.8 Hz, 2H), 1.47 (m, 18H), 1.29 (d, *J* = 6.8 Hz, 6H), 1.17 (t, *J* = 7.0 Hz, 6H).

^{77}Se{^{1}H}-NMR ($CDCl_3$, T=298K, ppm): δ 92.6.

^{13}C{^{1}H}-NMR ($CDCl_3$, T=298K, ppm): δ 208.7 (carbene), 148.9, 148.6, 146.5, 146.2, 134.2, 133.7, 132.8, 130.3, 129.9, 129.9, 128.6, 128.0, 127.4, 124.7, 124.6, 124.5, 124.2, 124.1, 122.7, 99.7, 99.7, 77.4, 77.2, 77.0, 76.6, 66.8, 66.7, 28.6, 28.5, 28.5, 25.7, 25.6, 25.2, 25.1, 24.0, 23.9, 23.9, 15.1.

Elemental analysis calcd (%) for $C_{37}H_{51}AuN_2O_2Se$: C, 53.43; H, 6.18; N, 3.37, found: C, 53.11; H, 6.30; N, 3.41.

Synthesis of complex 11b



In a 10 mL vial equipped with a stir-bar, 61.0 mg of **7b** (0.07 mmol), 17.3 mg of elemental selenium (0.22 mmol), and 4 mL of anhydrous toluene were added under argon atmosphere. The solution was stirred at 110°C for 24 hours. During the reaction the solution change to light orange. Afterwards, the solvent was removed and dichloromethane was added. Elemental selenium was eliminated by filtration on PTFE microfilter and the filtrate was concentrated and precipitated with pentane.
This process afforded 43.3 mg of **11b** (yield = 66%) as an orange solid.

^{1}H NMR (300 MHz, $CDCl_3$, T=298K, ppm): δ 7.48 (t, *J* = 7.7 Hz, 2H), 7.26 (m, *J* = 4.8 Hz, 3H), 7.23-7.04 (m, 2H), 6.95-6.86 (m, 2H), 5.04 (s, 2H), 3.55-3.36 (m, 6H), 3.05 (td, *J* = 6.9, 2.8 Hz, 2H), 1.61-1.23 (m, 24H), 1.17 (t, *J* = 7.0 Hz, 6H)
^{77}Se{^{1}H}-NMR ($CDCl_3$, T=298K, ppm): δ 113.6.
^{13}C{^{1}H}-NMR ($CDCl_3$, T=298K, ppm): δ 208.2 (carbene), 175.0, 148.9, 148.8, 146.6, 146.4, 140.4, 140.2, 134.2, 133.1, 132.7, 130.1, 129.7, 129.1, 126.3, 126.0, 125.7, 125.4, 125.1, 124.8, 124.5, 124.4, 124.3, 124.0, 123.9, 123.9, 123.8, 123.8, 123.6, 122.5, 122.4, 122.4, 99.8, 99.8, 99.7, 77.3, 77.0, 76.7, 66.8, 66.4, 28.6, 28.6, 28.5, 25.6, 25.6, 25.2, 23.9, 23.9, 23.9, 23.7, 15.1, 15.1.
Elemental analysis calcd (%) for $C_{38}H_{50}AuF_3N_2O_2Se$: C, 50.73; H, 5.60; N, 3.11, found: C, 50.40; H, 5.78; N, 3.22.

Biological data

Cell Culture

Human breast adenocarcinoma cells (MCF-7), human pancreas adenocarcinoma cells (PT45) and human ovarian carcinoma (HeLa) cells were cultured in DMEM medium (4.5 g/L D-Glucose, L-Glutamine) supplemented with 10% FBS Superior, 2.4% penicillin/streptomycin, 1.2% GlutaMAX-I and 1% sodium pyruvate. Human fibroblasts (GM-5657) cells were cultured in DMEM medium (1 g/L D-Glucose) supplemented with 10% FBS Superior, 2.4% penicillin/streptomycin, 1.2% GlutaMAX-I and 1% sodium pyruvate. LGC Standards Ltd. provided all the cell lines, which were cultured at 37 °C with 10% CO_2. Prior to each experiment, the cells were passaged at least 3 times.

Distribution Coefficient

The lipophilicity of the metal complexes was determined by measuring its distribution coefficient between the phosphate-buffered saline and Octanol phase by using the "shake-flask" method. For this technique, the used phases were previously saturated in each other (45mL of phase 1 in 5 mL of phase 2). The complex was dissolved in the phase 1 with its presence calculated using lambert-Beer equation. This solution was then mixed with an equal volume of the other phase (2) at 300 rpm for 12 h and then equilibrated overnight. The phase 1 was then carefully separated from phase 2. The amount of the complex before and after the sample mixing was determined by UV/Vis absorption spectroscopy at specific wavelength using a Jasco V-670 spectrophotometer. The evaluation of the complexes was repeated three times and the ratio between the organic and aqueous phase calculated.

Cytotoxicity Assay

A total of 6×10^3 cells were seeded onto 96-well plates and allowed to adhere overnight. The cells were treated with increasing concentrations of the metal complex diluted in cell media achieving a total volume of 200 µL for 48 h at 37 °C and 10% CO_2. After this time, 50 µL of phosphate-buffered saline buffer containing 3-(4,5-Dimethylthiazol-2-yl)-2,5-diphenyltetrazolium bromide (MTT) was added. The cells were incubated for 2 h at 37 °C and 10% CO_2 and the mixture was replaced by 200 µL DMSO.

Fluorescence Staining of the Reactive Oxygen Species Generation

A total of 2.5×10^5 cells were seeded onto 8-well plate and allowed to adhere overnight. The cells were treated with the metal complex which was diluted in cell media to a total volume of 200 µL for 4 h. To assess the generation of reactive oxygen species, the cells were incubated with phosphate-buffered saline buffer containing 2',7'- dichlorodihydrofluorescein diacetate with a final concentration of 15 µM at 37 °C and 10% CO_2 for 30 minutes and imaged by fluorescence microscopy. The camera was

mounted on an Olympus IX81 inverted fluorescence microscope equipped with various fluorescence filter. All images were recorded with a 10x objective and 1x ocular. λ_{ex} = 460-490 nm, λ_{em} = 517-527 nm.

Dual fluorescence cell viability staining

A total of 2.5 × 10^5 cells were seeded onto 8-well plate and allowed to adhere overnight. The cells were treated with the metal complex which was diluted in cell media to a total volume of 200 µL for 24 h. To assess the viability of the cells, phosphate-buffered saline buffer containing Calcein-AM at a final concentration of 2 µM was used to dye the cells. The cells were incubated at 37 °C with 10% CO_2 for 30 min. After this time the phosphate-buffered saline buffer containing Calcein-AM was discharged, the cells were washed three times with phosphate-buffered saline buffer and phosphate-buffered saline buffer containing Propidium iodide was added at a final concentration of 0.5 µM. The cells were incubated at room temperature for 5 min and imaged by fluorescence microscopy. The camera was mounted on an Olympus IX81 inverted fluorescence microscope equipped with various fluorescence filter. All images were recorded with a 10x objective and 1x ocular. Calcein-AM: λ_{ex} = 460-490 nm, λ_{em} = 517 nm. Propidium iodide: λ_{ex} = 545-580 nm, λ_{em} = 617 nm.

Depletion of glutathione by fluorescence microscopy

A total of 2.5 × 10^5 cells were seeded onto 8-well plate and allowed to adhere overnight. The cells were treated with the metal complex which was diluted in cell media to a total volume of 200 µL for 6 h. To visualize the presence of glutathione, the cells were incubated with phosphate-buffered saline buffer containing ThiolTracker™ Violet (20 µM) at 37 °C with 10% CO_2 for 30 min and imaged by fluorescence microscopy. The camera was mounted on an Olympus IX81 inverted fluorescence microscope equipped with various fluorescence filter. All images were recorded with a 10x objective and 1x ocular. λ_{ex} = 330-385 nm, λ_{em} = 526 nm.

Generation of Lipid Peroxides by Fluorescence Microscopy

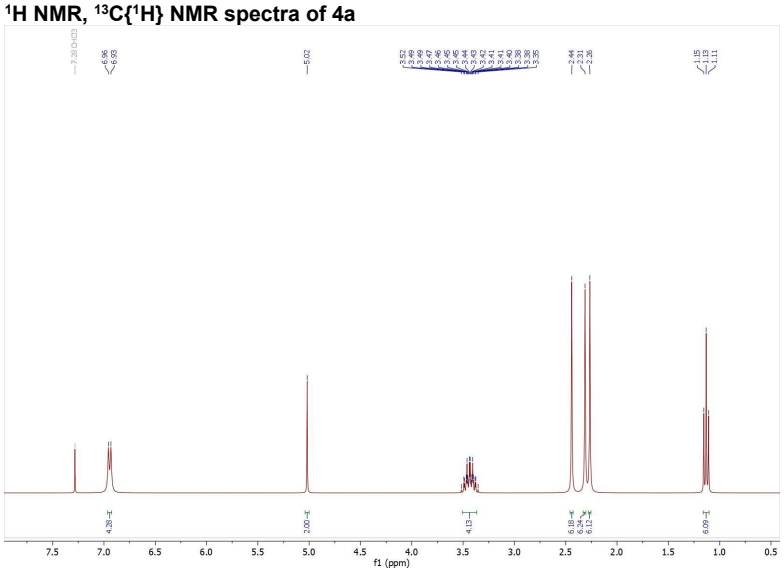
A total of 2.5 × 10^5 cells were seeded onto 8-well plate and allowed to adhere overnight. The cells were treated with the metal complex which was diluted in cell media to a total volume of 200 µL for 4 h. To assess the generation of lipid peroxides, the cells were incubated with phosphate-buffered saline buffer containing BODIPY581/591 C11 (5 µM) at 37 °C and 10% CO_2 for 30 min and imaged by fluorescence microscopy. The camera was mounted on an Olympus IX81 inverted fluorescence microscope equipped with various fluorescence filter. All images were recorded with a 10x objective and 1x ocular. λ_{ex} = 460-490 nm, λ_{em} = 510 nm.

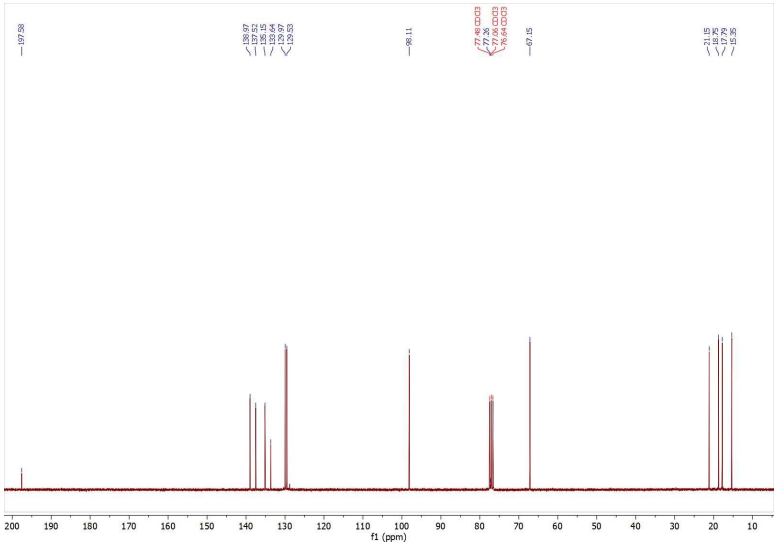
Cell fluorescent imaging of intracellular Fe^{2+} by fluorescence microscopy

A total of 2.5×10^5 cells were seeded onto 8-well plate and allowed to adhere overnight. The cells were treated with the metal complex which was diluted in cell media to a total volume of 200 μL for 6 h. To assess the viability of the cells, phosphate-buffered saline buffer containing BioTracker™ FerroOrange at a final concentration of 1 μM was used to dye the cells. The cells were incubated at 37 °C with 10% CO_2 for 30 min and imaged by fluorescence microscopy. The camera was mounted on an Olympus IX81 inverted fluorescence microscope equipped with various fluorescence filter. All images were recorded with a 10x objective and 1x ocular. λ_{ex} = 460-490 nm, λ_{em} = 572 nm.

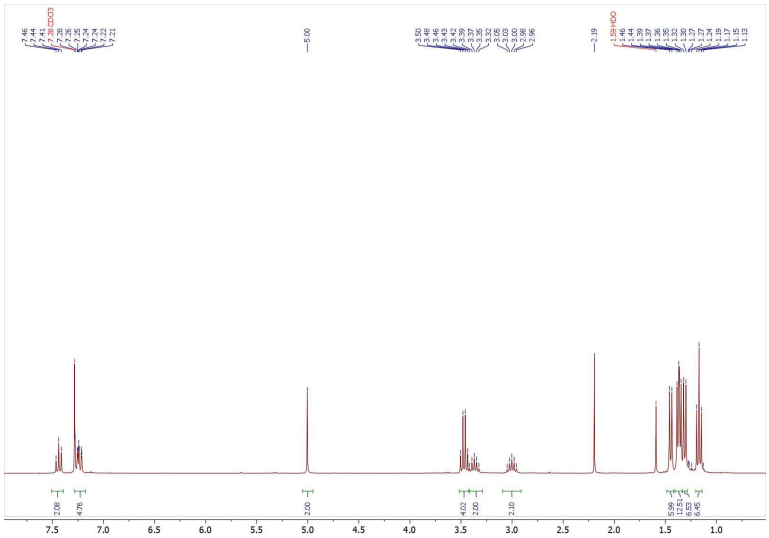
NMR spectra

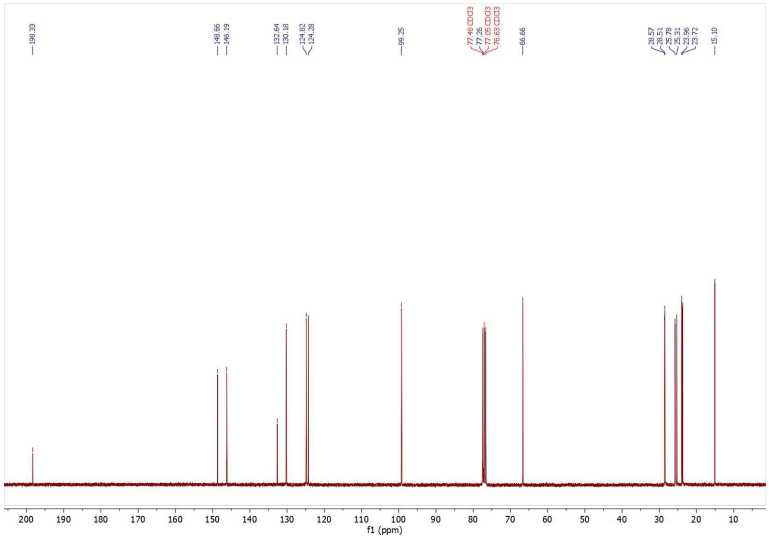
^{1}H NMR, ^{13}C{^{1}H} NMR spectra of 4a



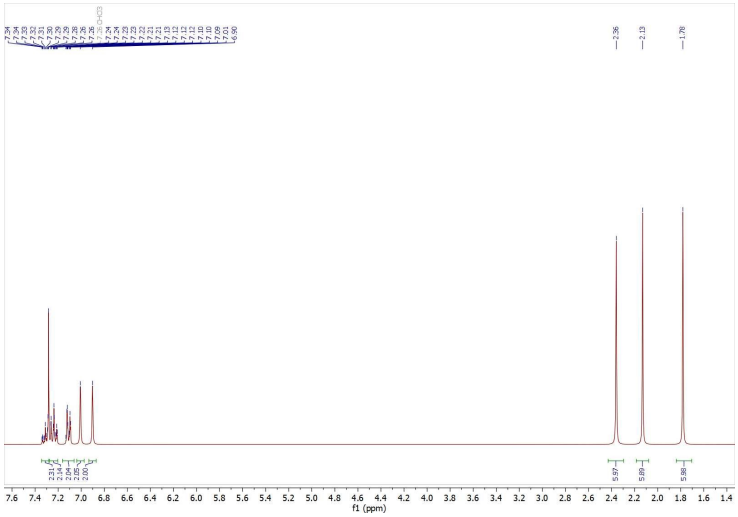


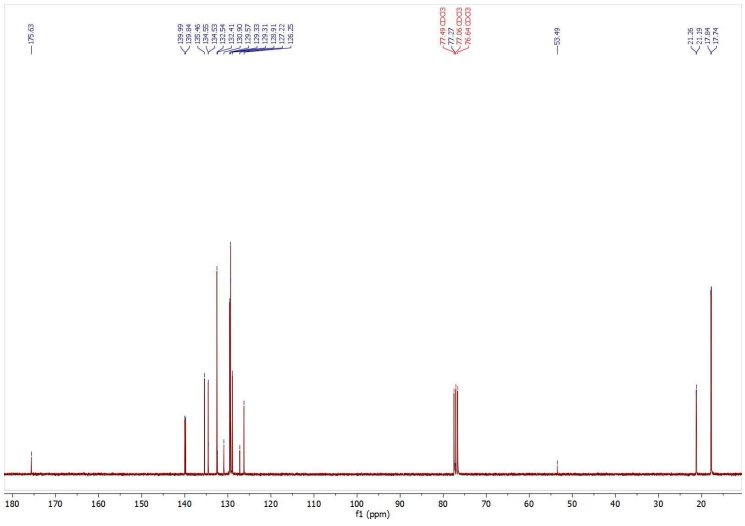
^{1}H NMR, ^{13}C{^{1}H} NMR spectra of 4b



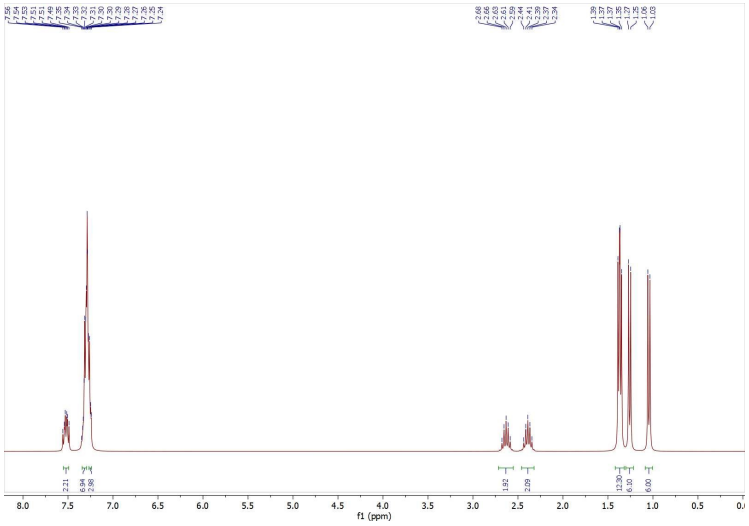


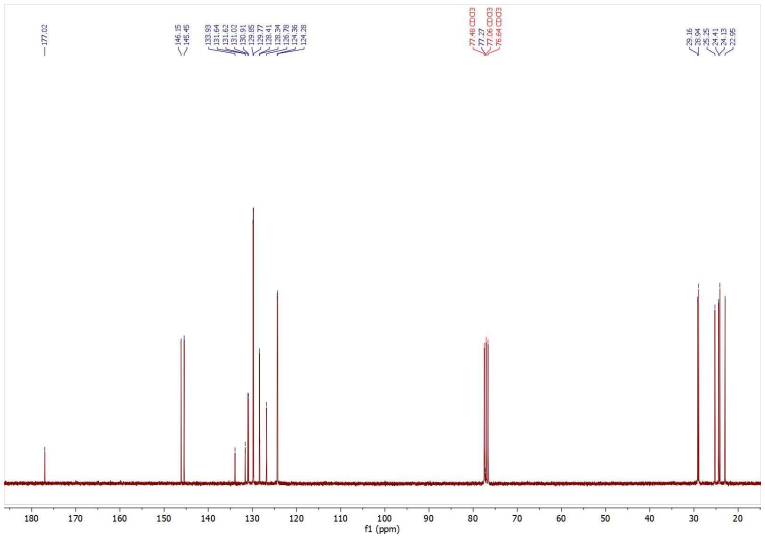
^{1}H NMR, ^{13}C{^{1}H} NMR spectra of 4c



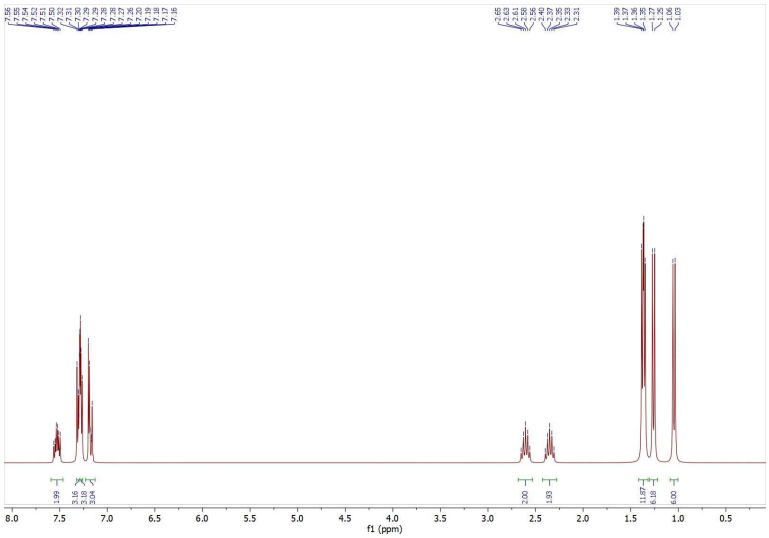


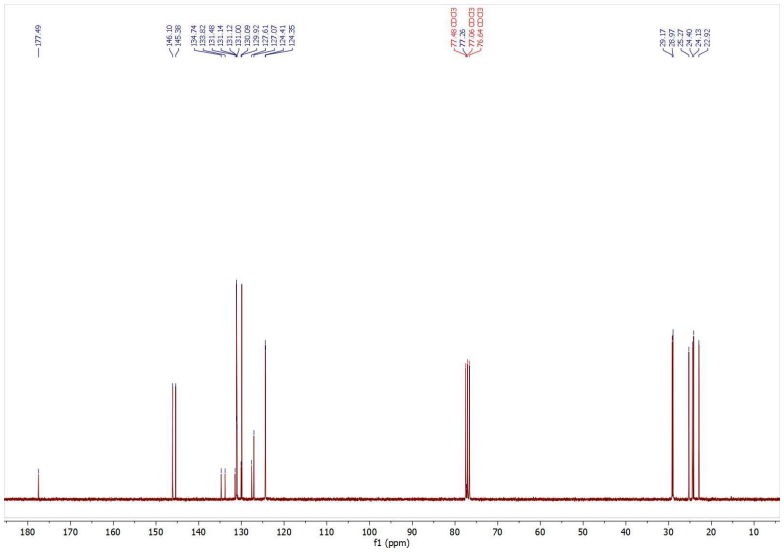
^{1}H NMR, ^{13}C{^{1}H} NMR spectra of 4d



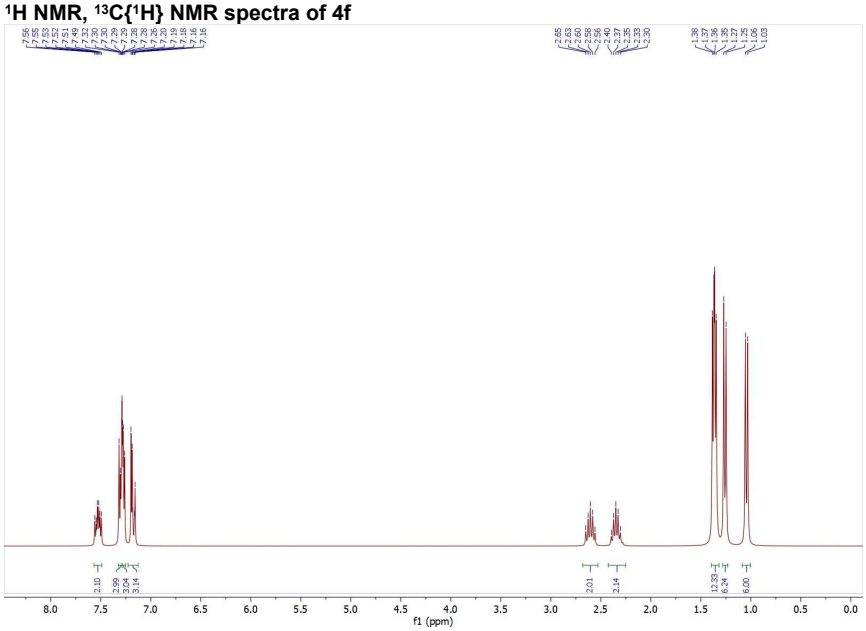


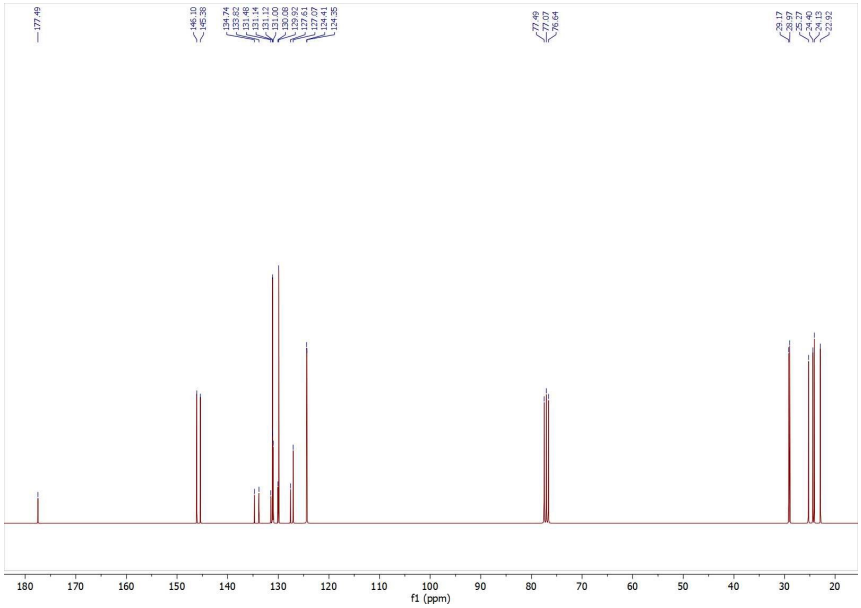
^{1}H NMR, ^{13}C{^{1}H} NMR spectra of 4e



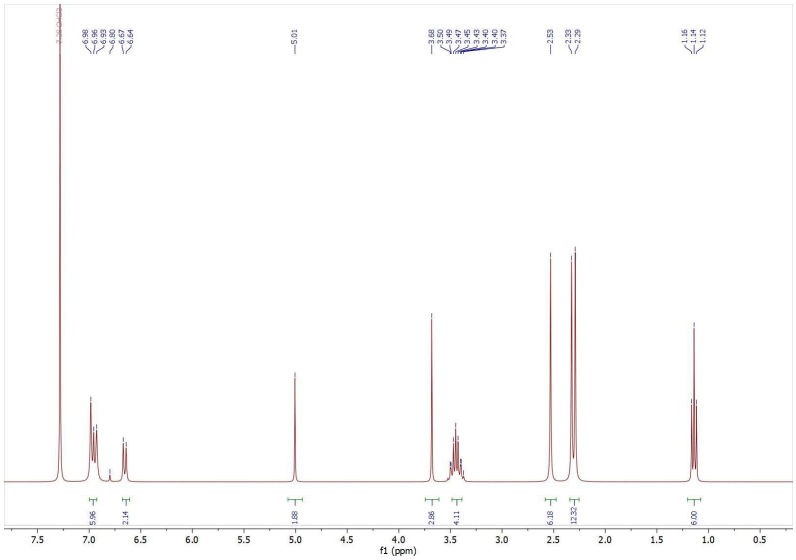


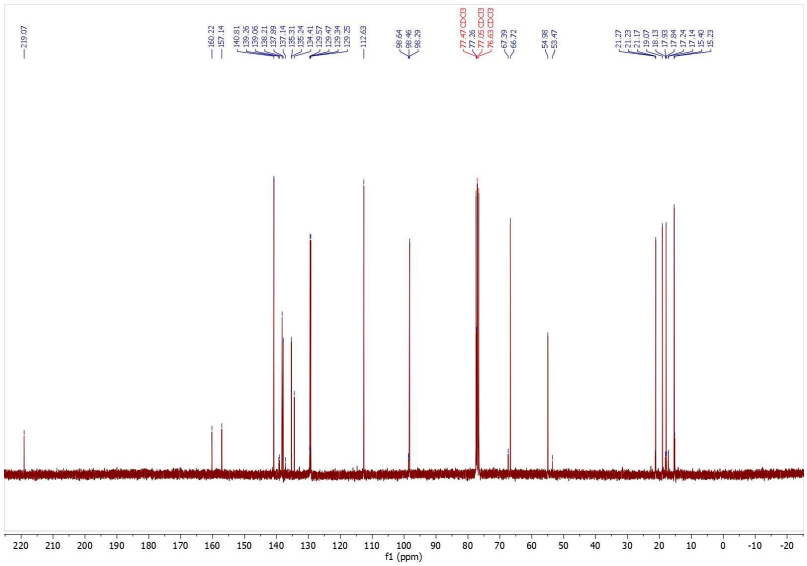
^{1}H NMR, ^{13}C{^{1}H} NMR spectra of 4f



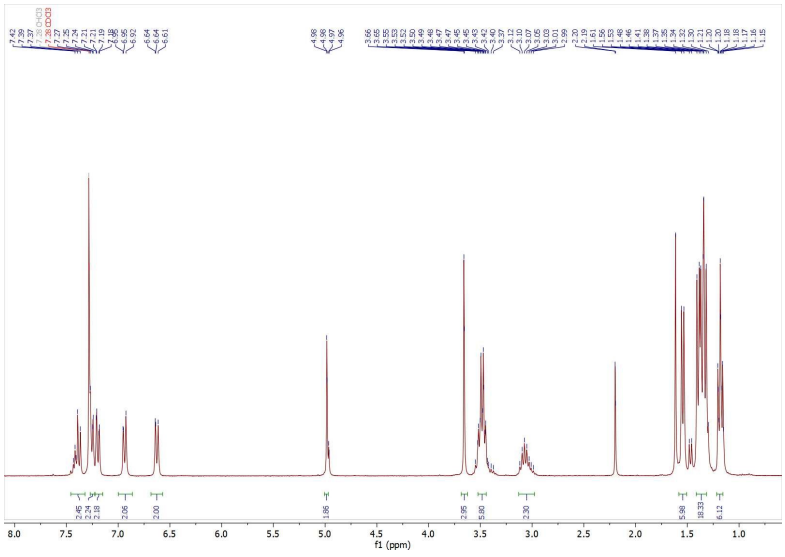


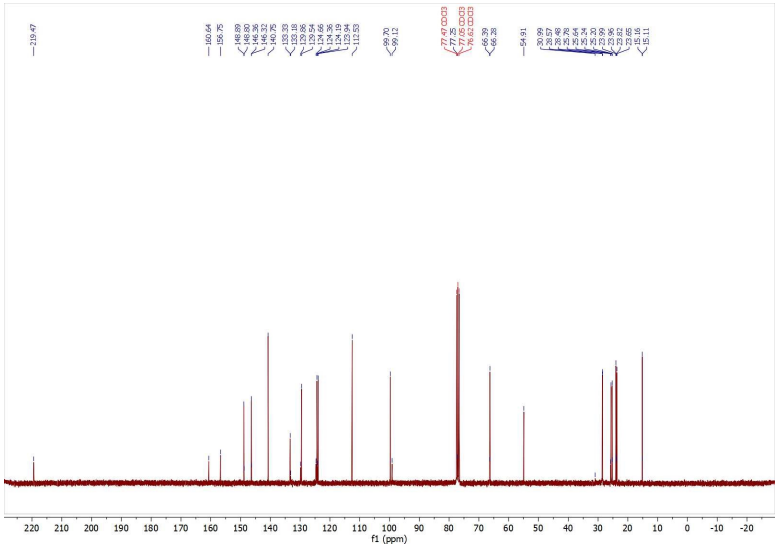
^{1}H NMR, ^{13}C{^{1}H} NMR spectra of 5a



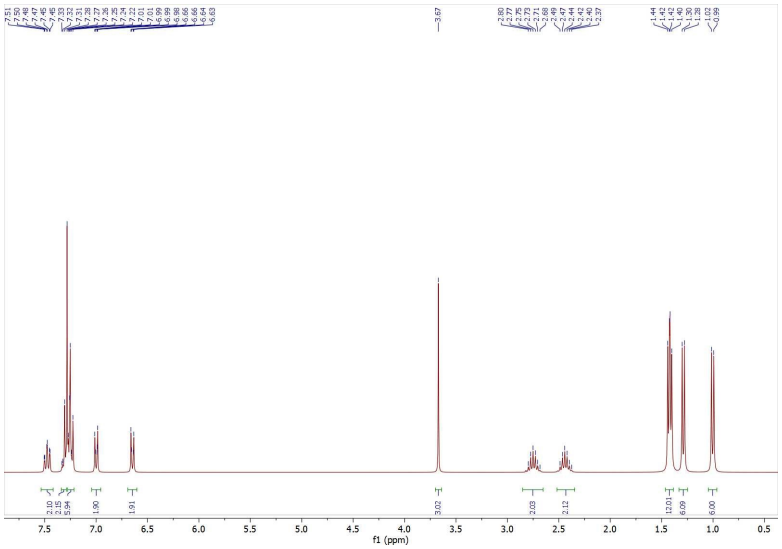


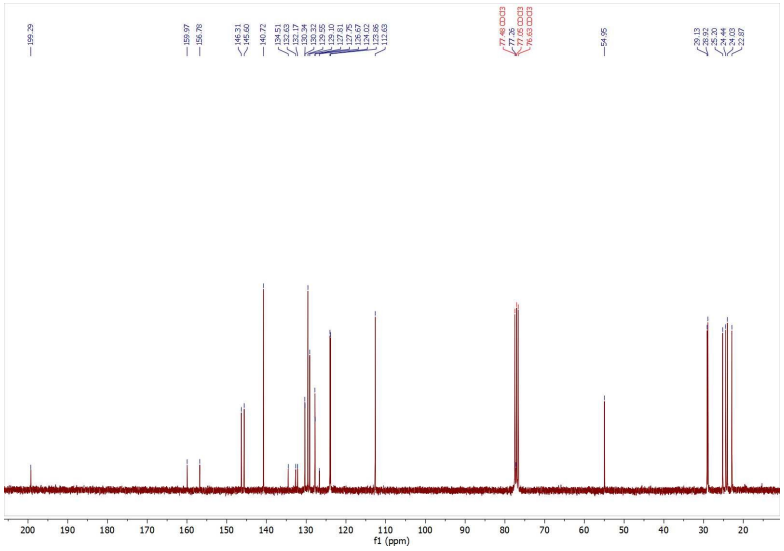
^{1}H NMR, ^{13}C{^{1}H} NMR spectra of 5b



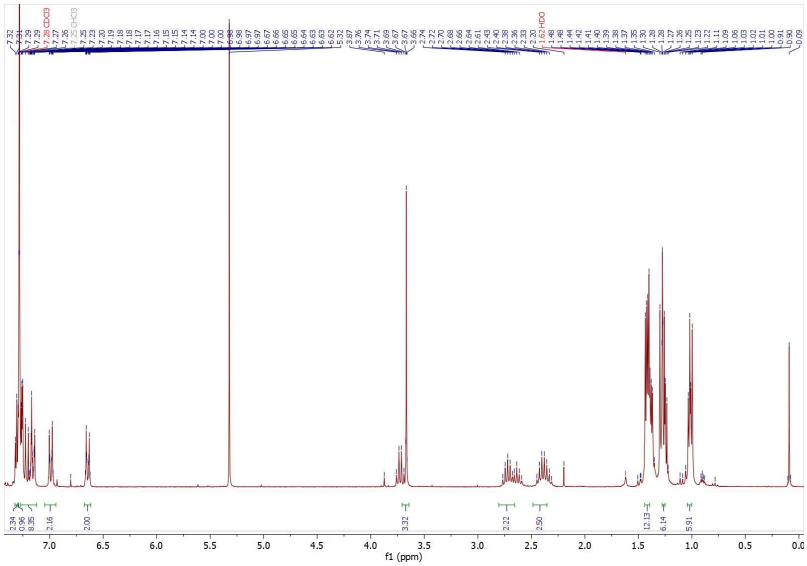


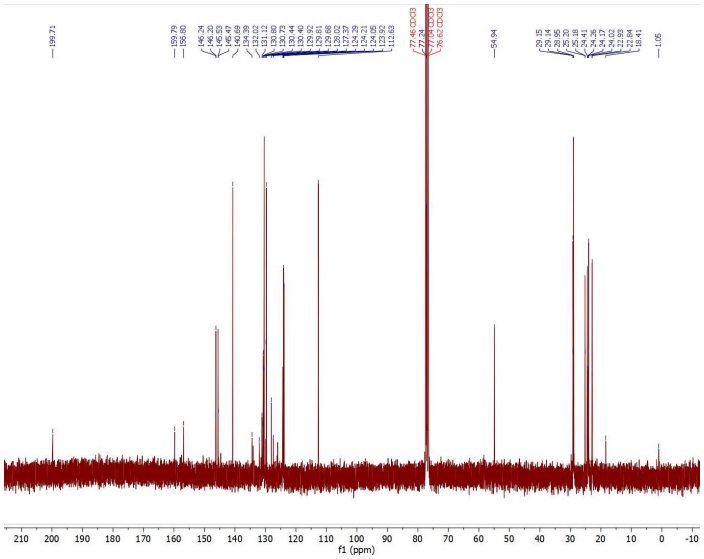
^{1}H NMR, ^{13}C{^{1}H} NMR spectra of 5d



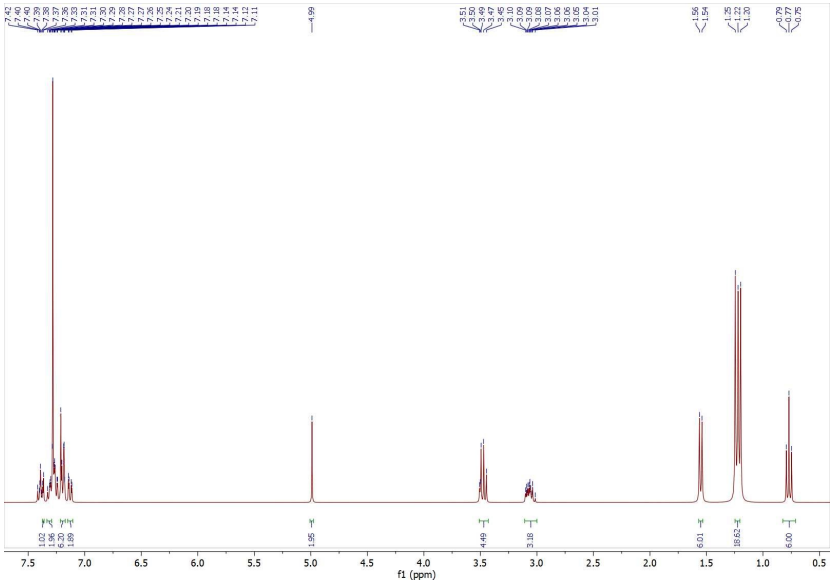


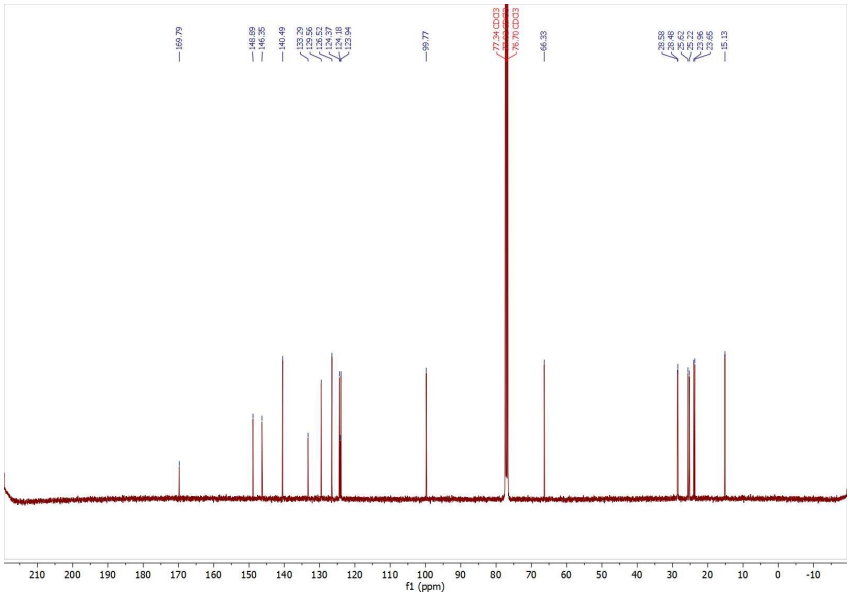
^{1}H NMR, ^{13}C{^{1}H} NMR spectra 5f



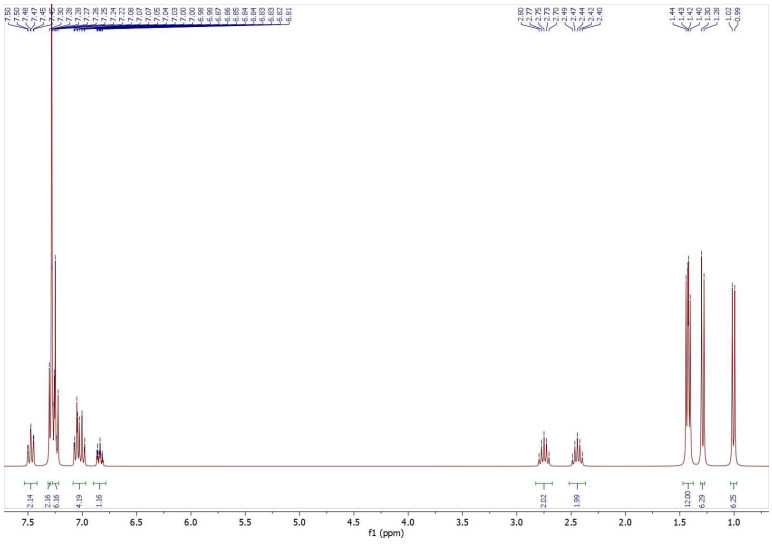


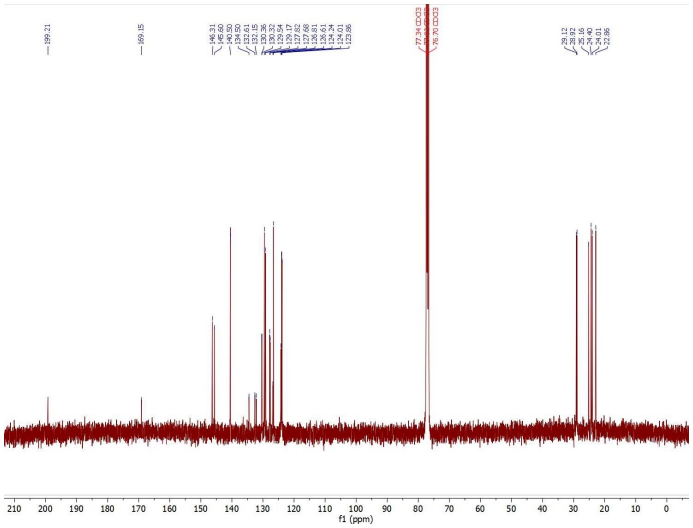
^{1}H NMR, ^{13}C{^{1}H} NMR spectra of 6b



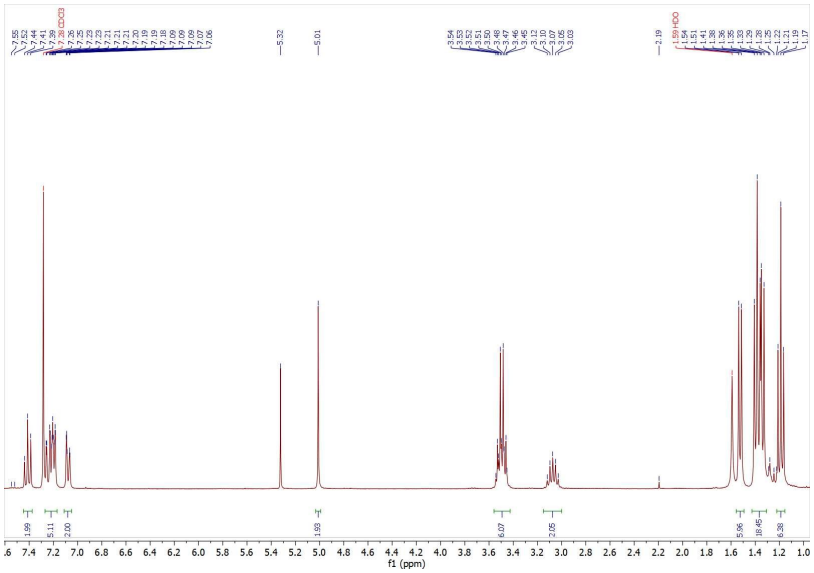


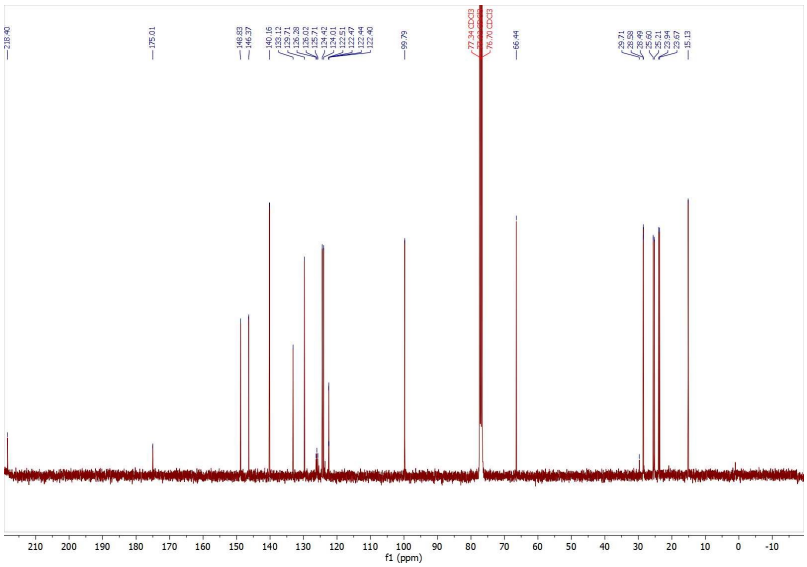
^{1}H NMR, ^{13}C{^{1}H} NMR spectra of 6d



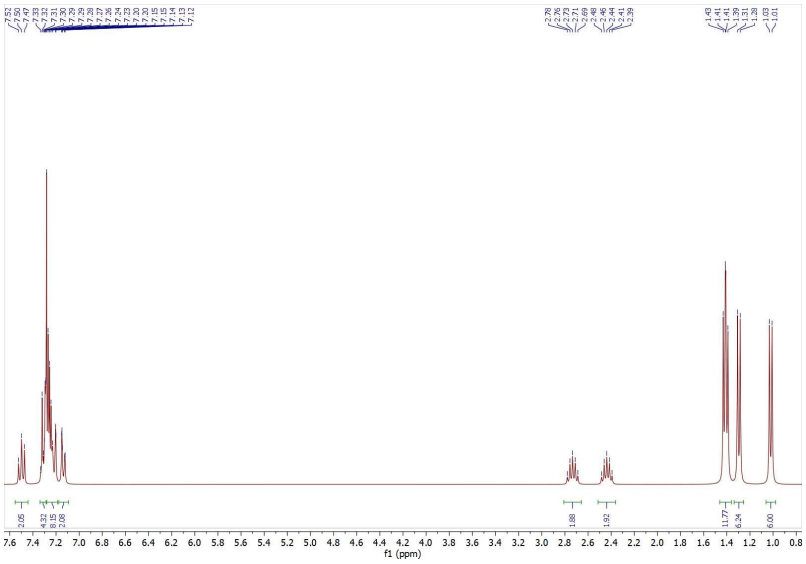


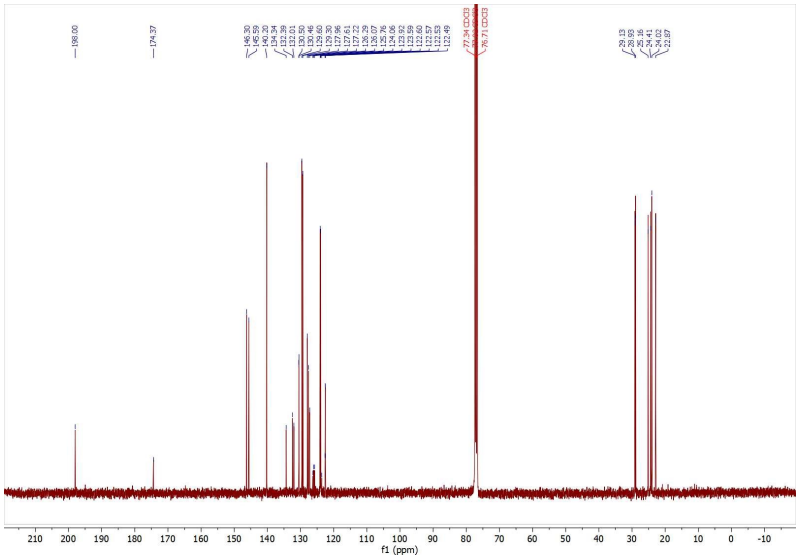
^{1}H NMR, $^{13}C\{^{1}H\}$ NMR spectra of 7b



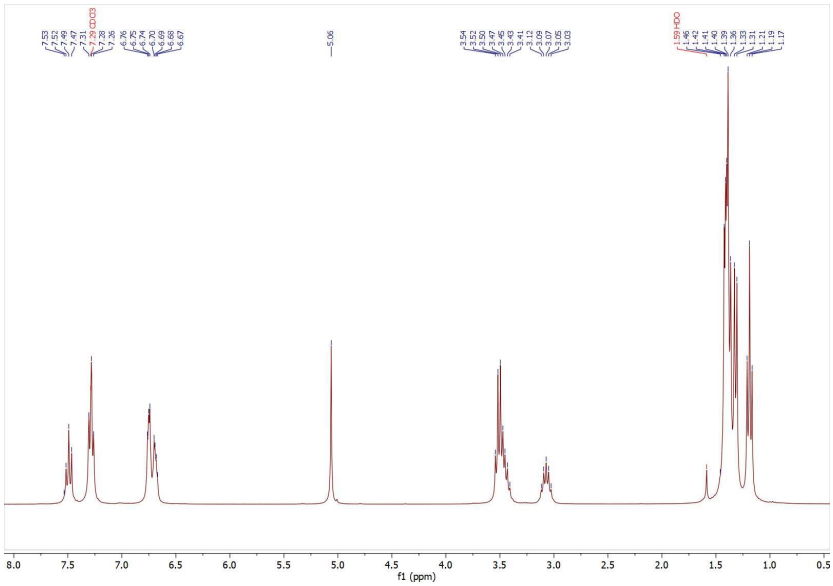


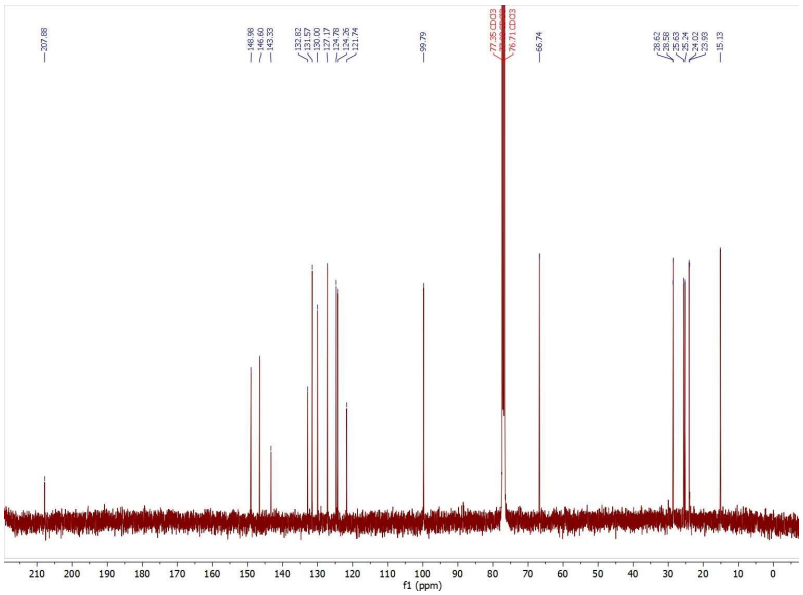
^{1}H NMR, ^{13}C{^{1}H} NMR spectra of 7d



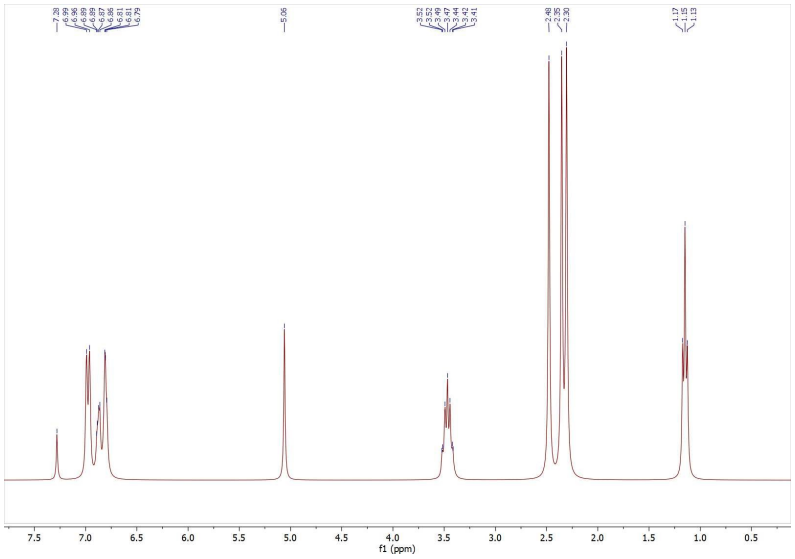


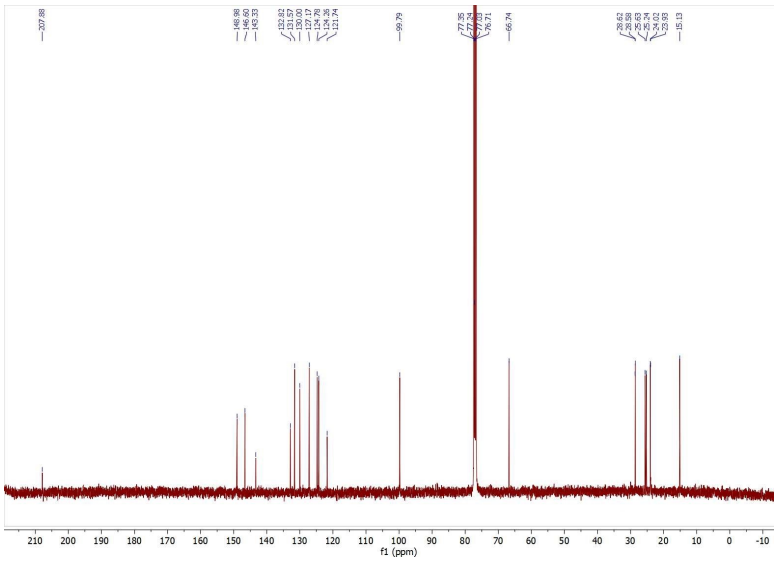
^{1}H NMR, ^{13}C{^{1}H} NMR spectra of 8a



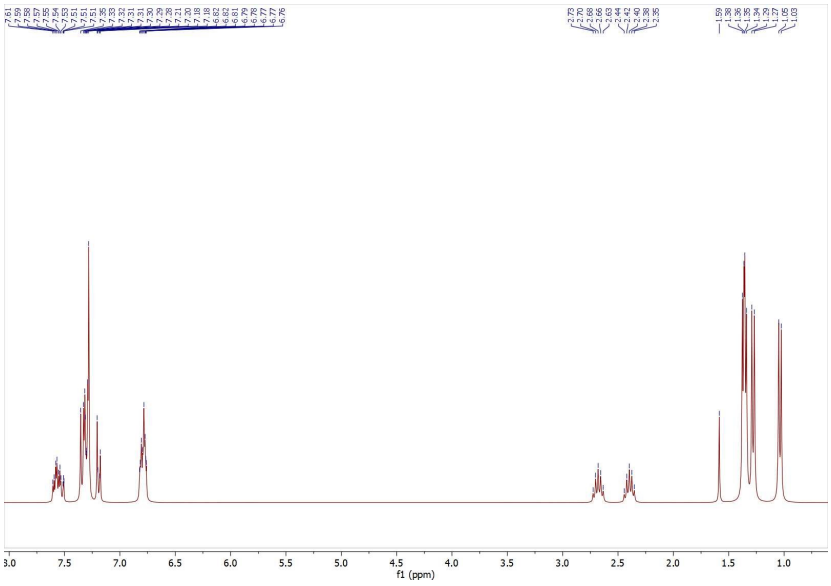


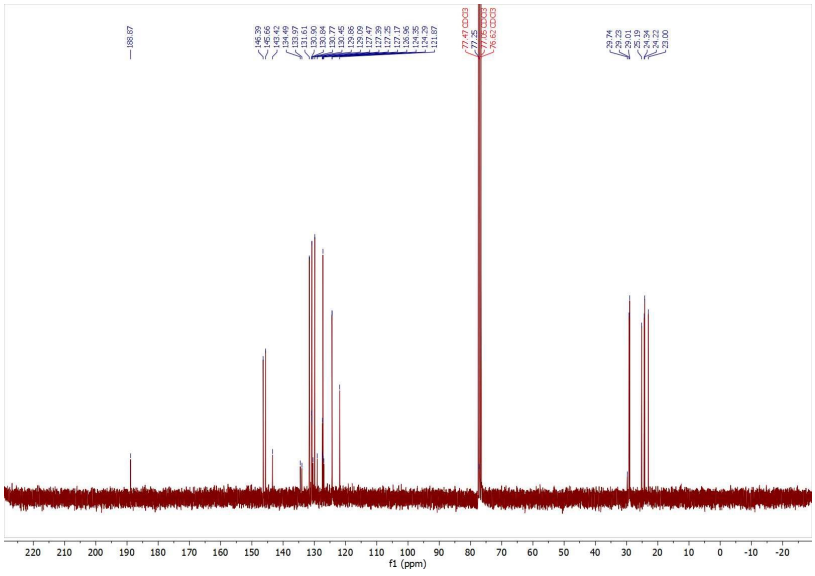
^{1}H NMR, $^{13}C\{^{1}H\}$ NMR spectra of 8b



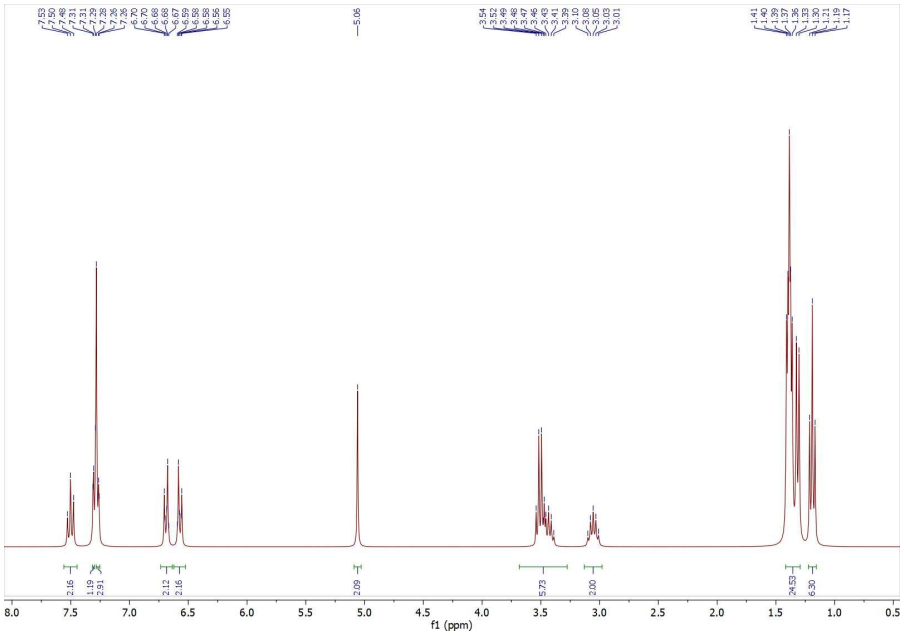


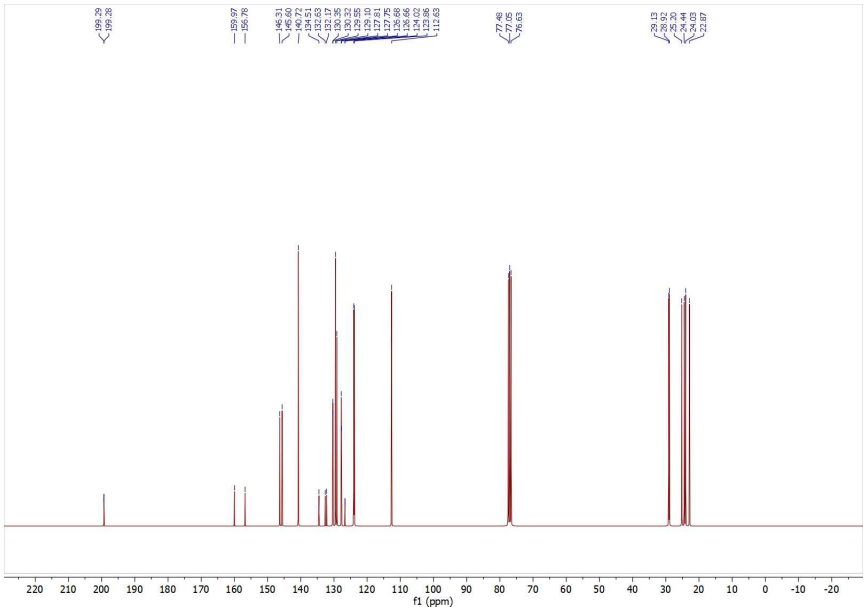
^{1}H NMR, ^{13}C{^{1}H} NMR spectra of 8f



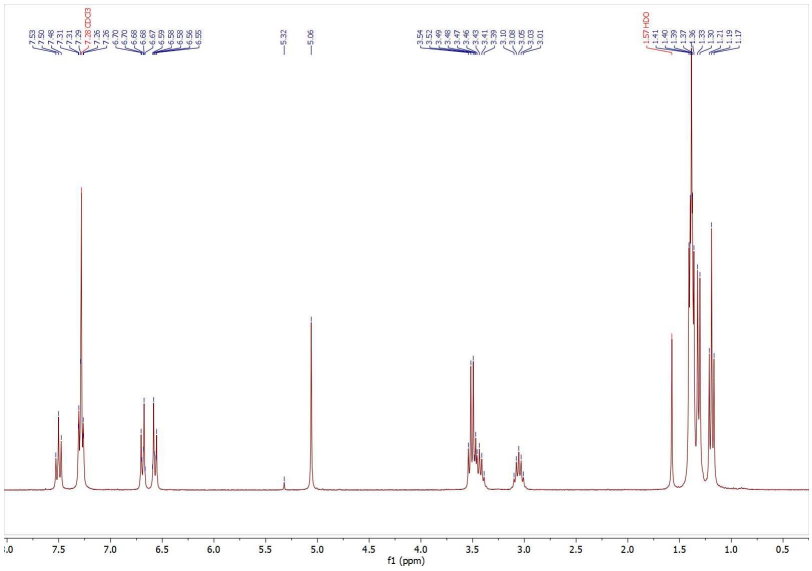


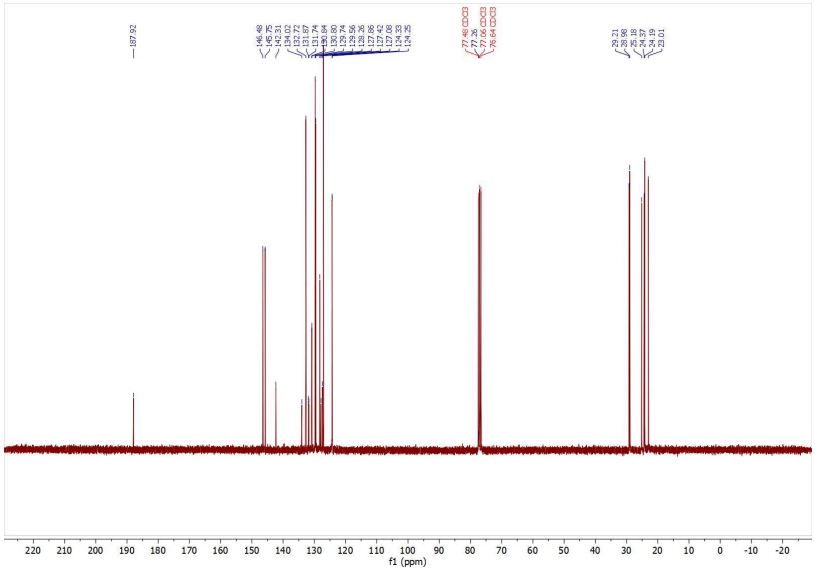
^{1}H NMR, ^{13}C{^{1}H} NMR spectra of 9b



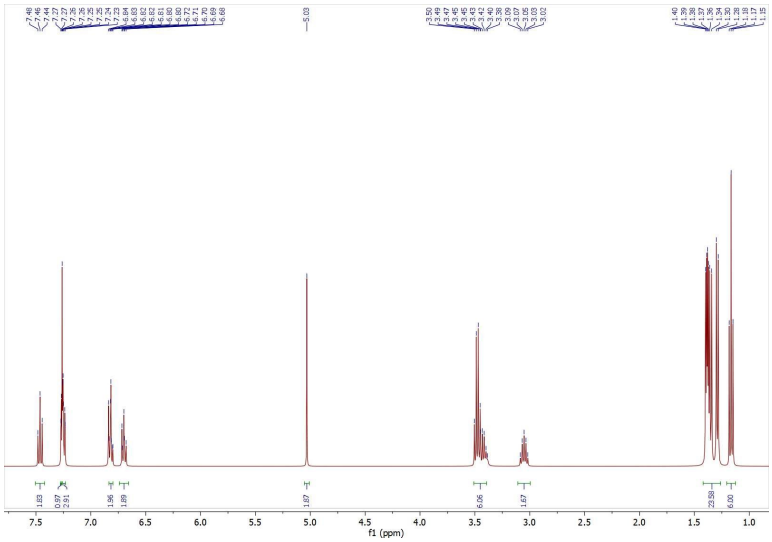


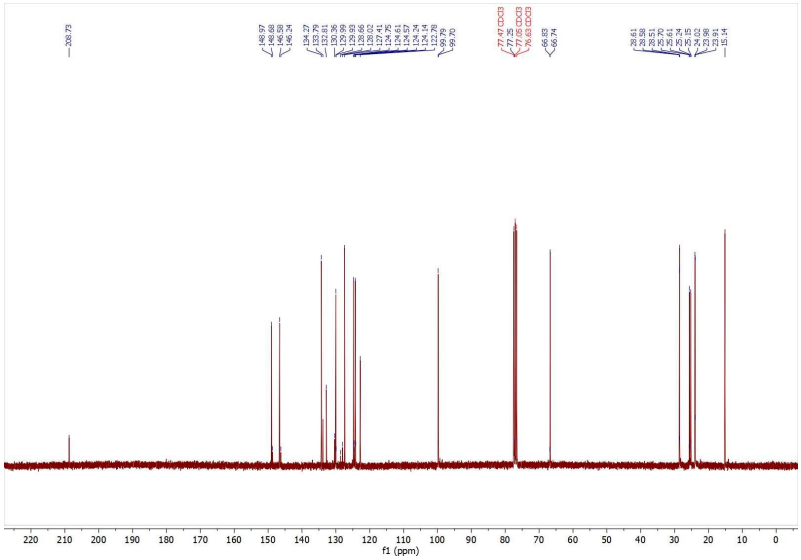
^{1}H NMR, ^{13}C{^{1}H} NMR spectra of 9d

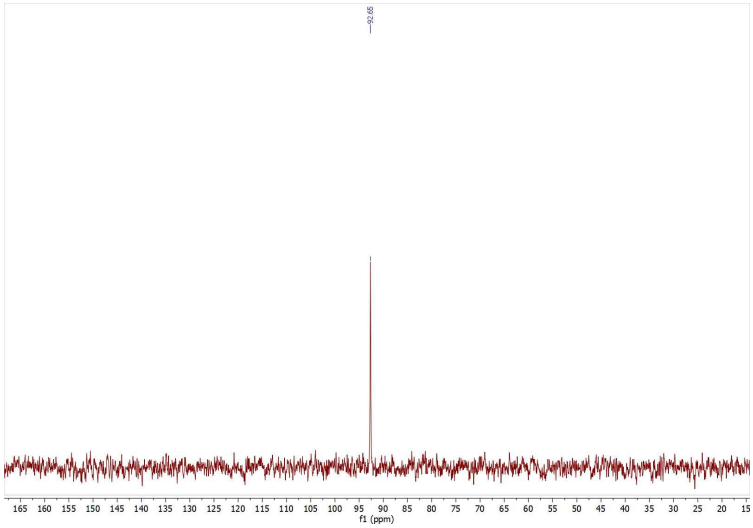




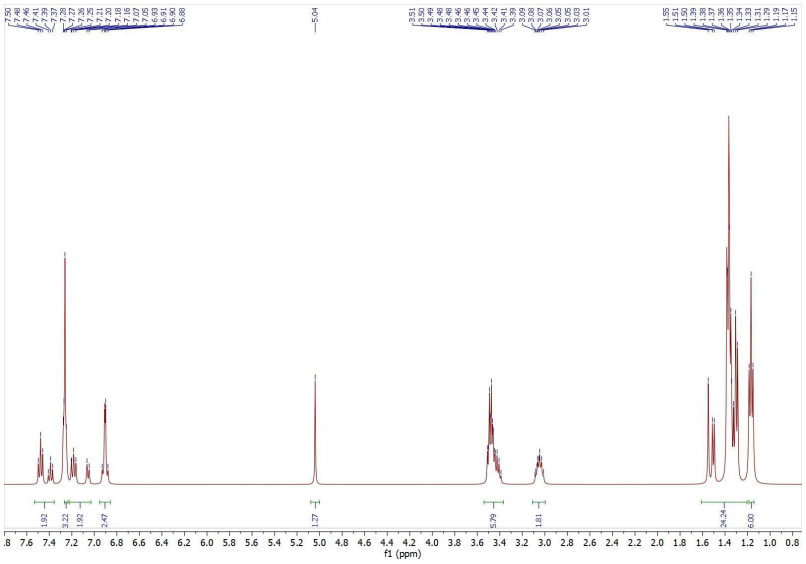
^{1}H NMR, ^{13}C{^{1}H} NMR and ^{77}Se{^{1}H} NMR spectra of 10b

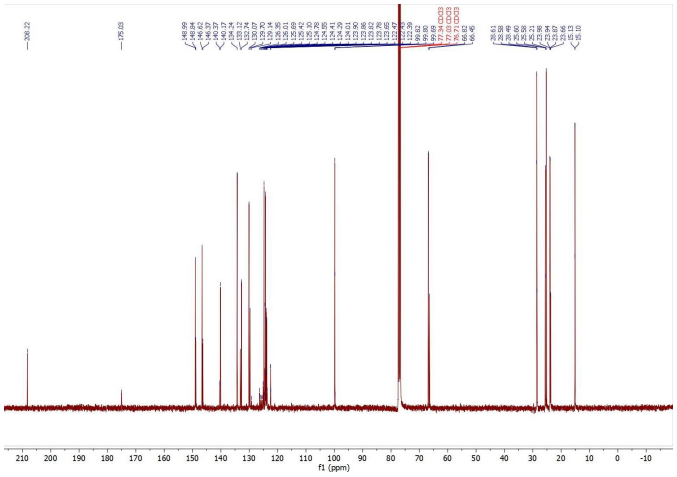


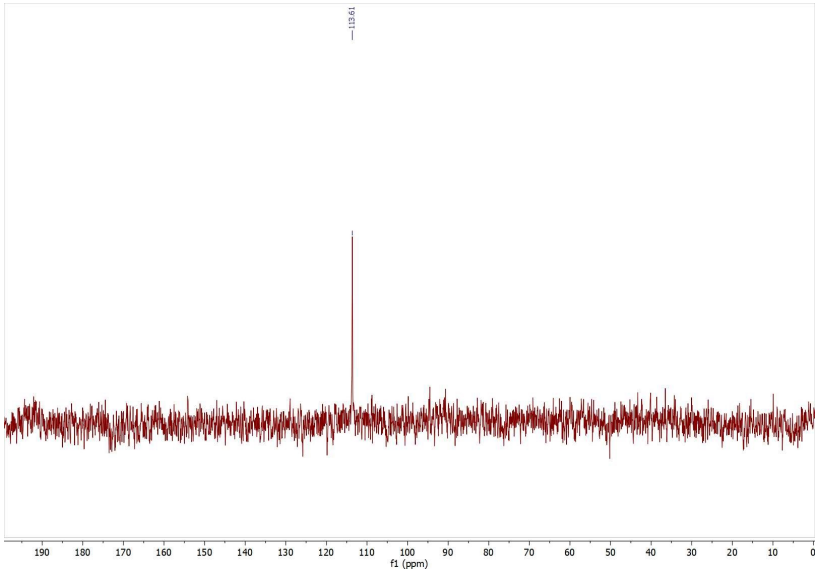




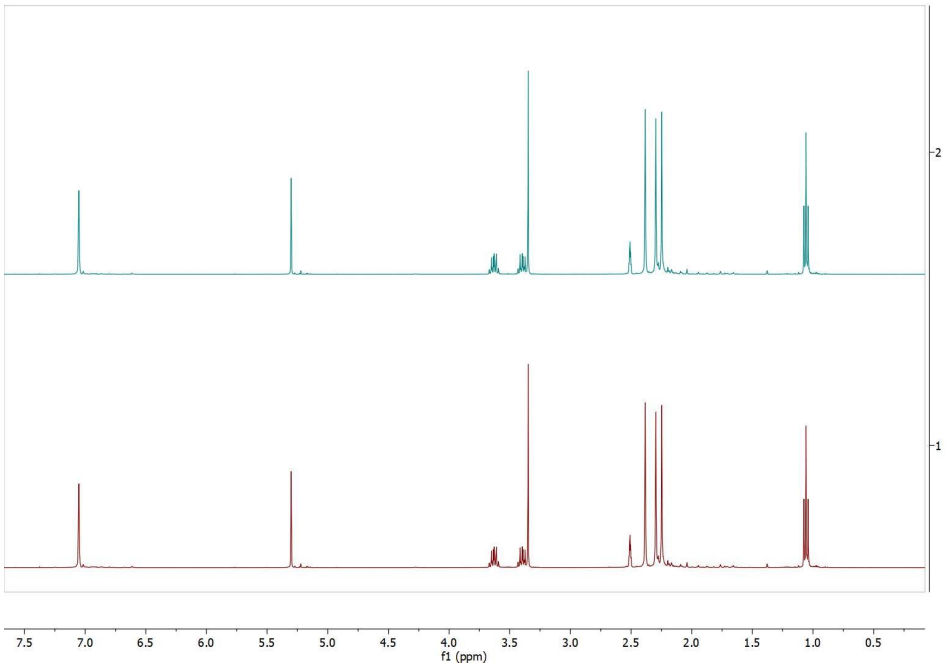
^{1}H NMR, ^{13}C{^{1}H} NMR and ^{77}Se{^{1}H} NMR spectra of 11b



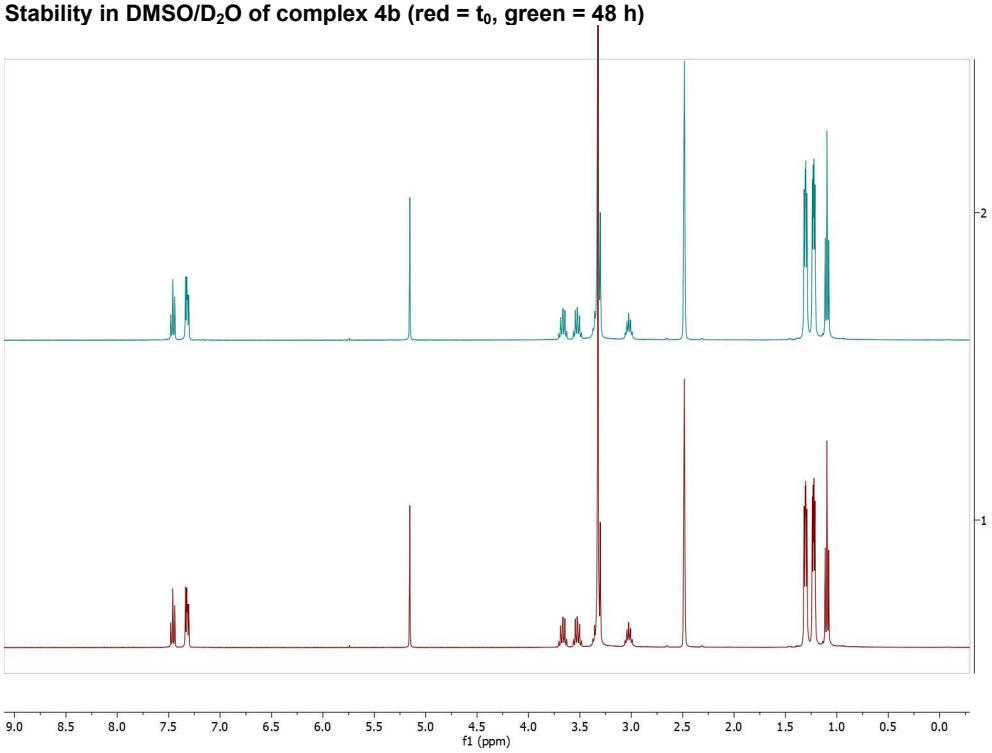




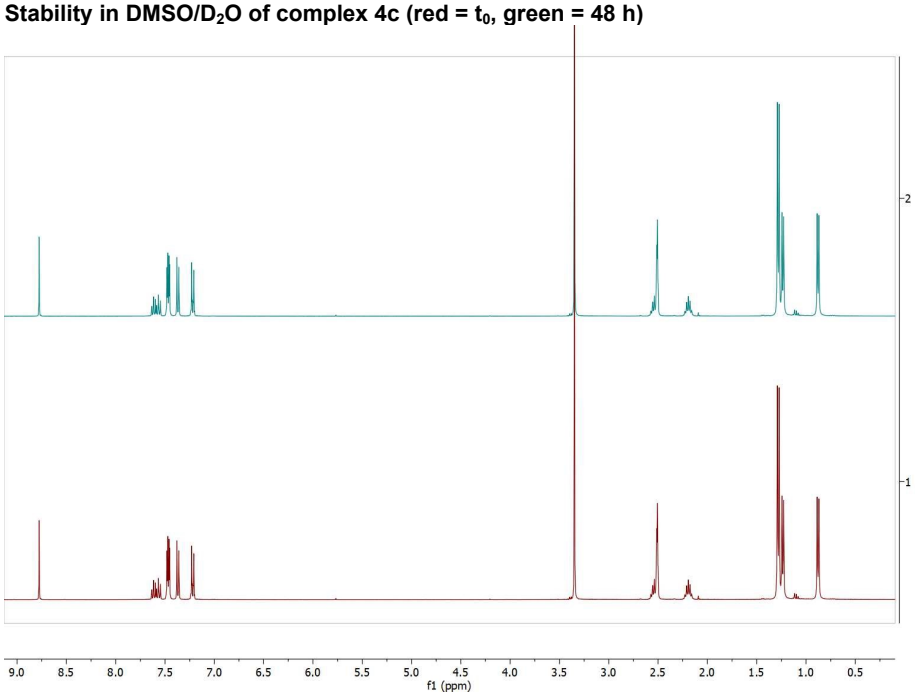
Stability in DMSO/D_2O of complex 4a (red = t_0, green = 48 h)



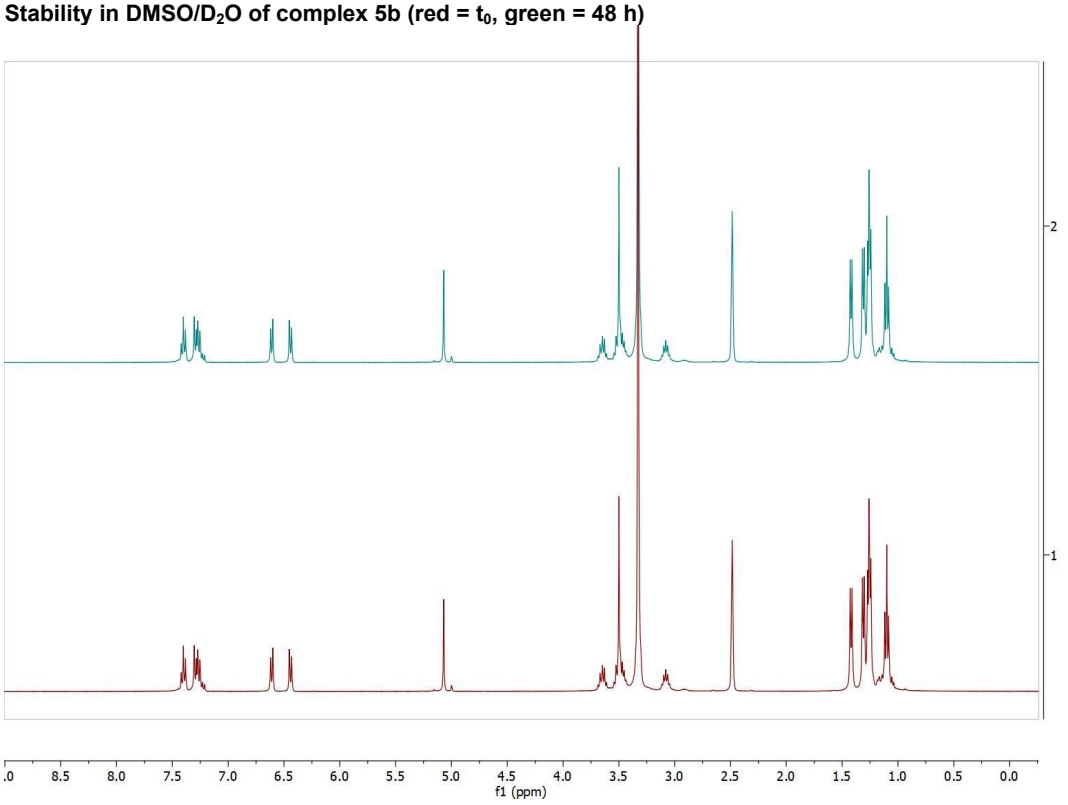
Stability in DMSO/D_2O of complex 4b (red = t_0, green = 48 h)



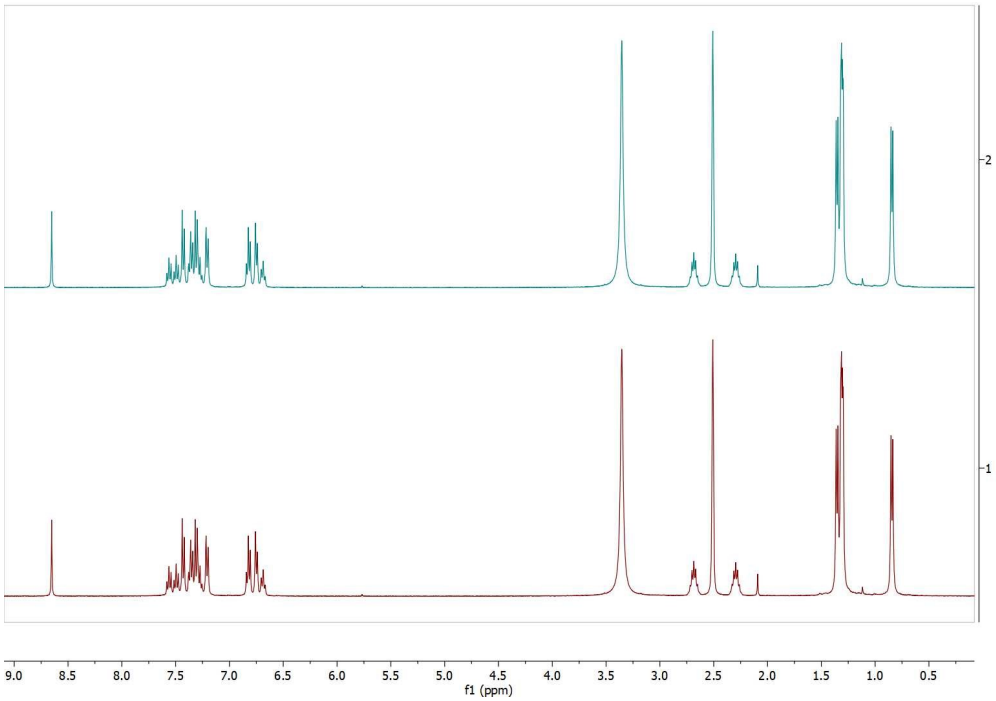
Stability in DMSO/D_2O of complex 4c (red = t_0, green = 48 h)



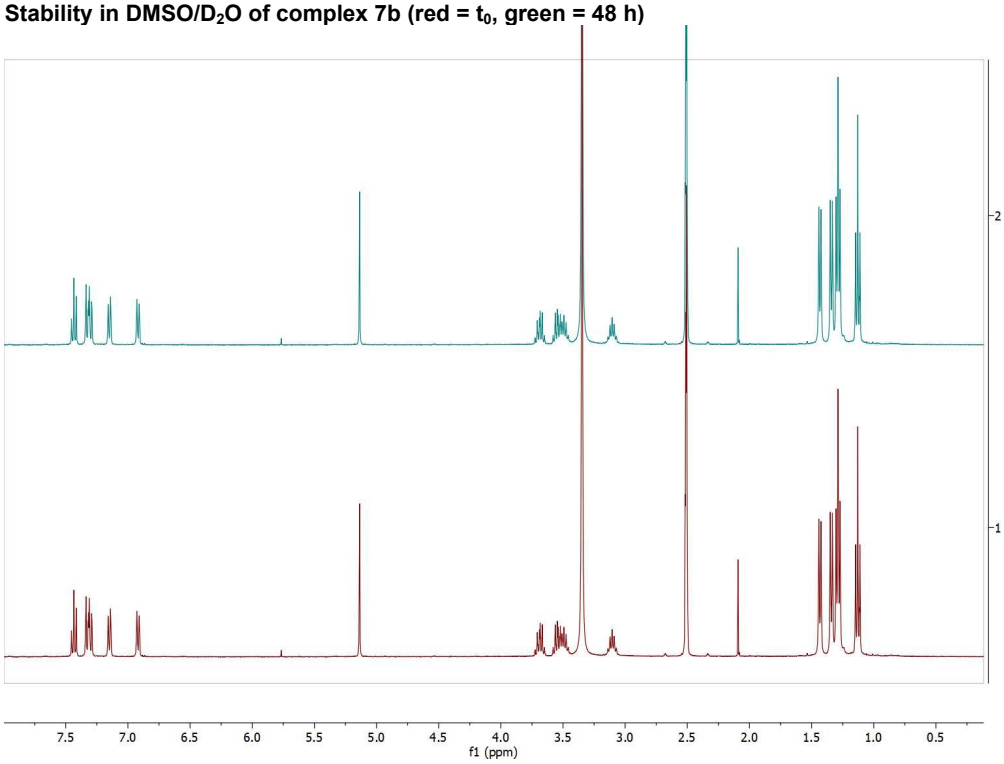
Stability in DMSO/D_2O of complex 5b (red = t_0, green = 48 h)



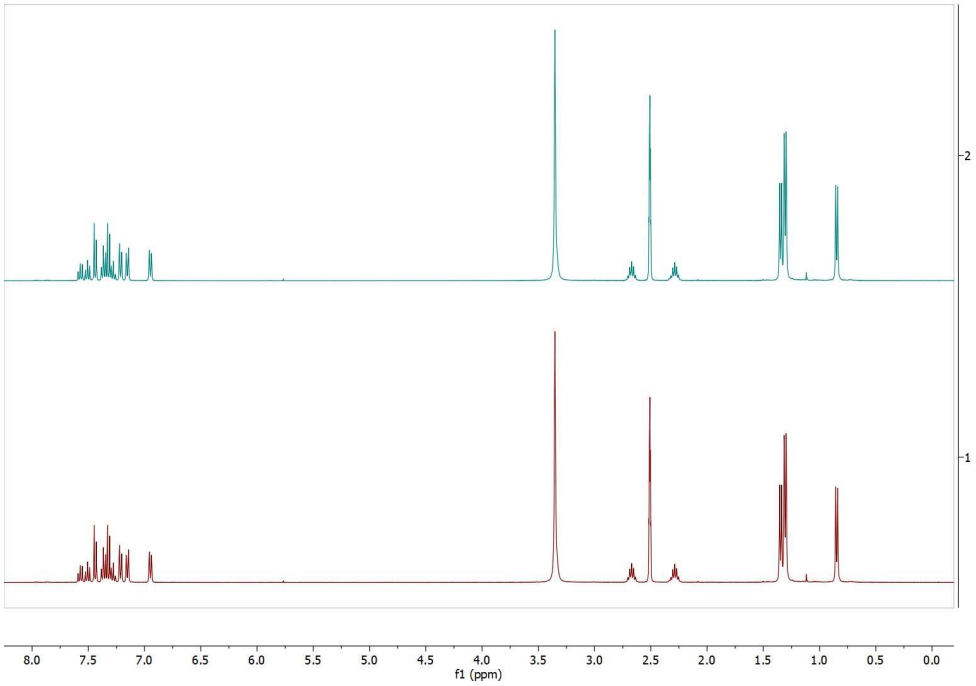
Stability in DMSO/D_2O of complex 6d (red = t_0, green = 48 h)



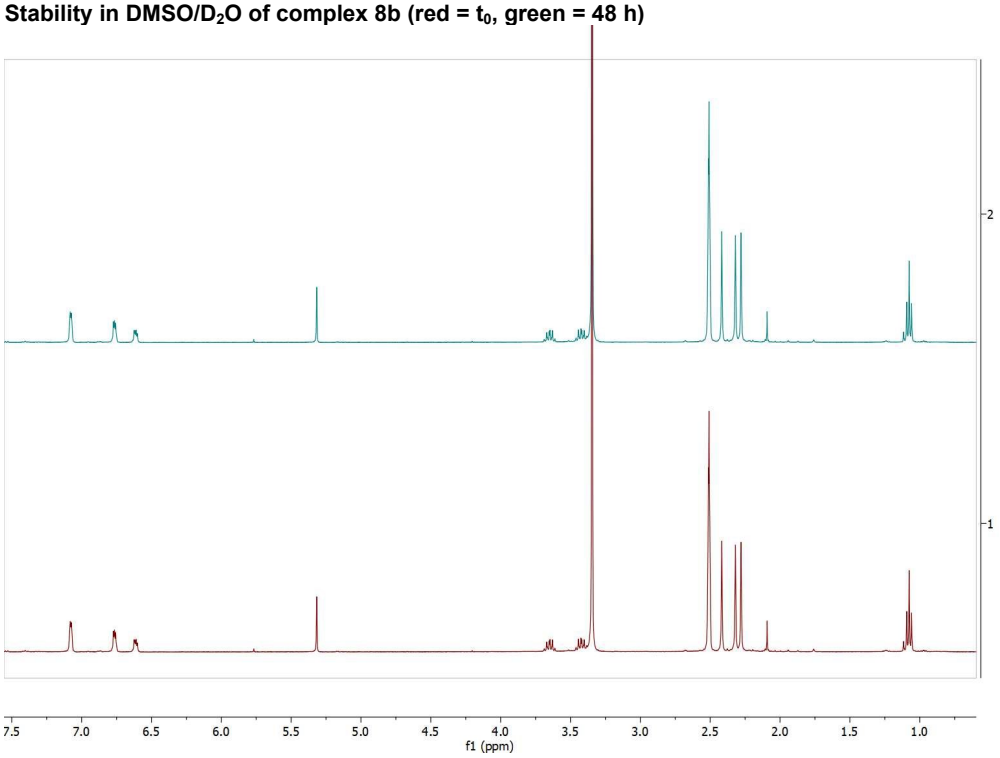
Stability in DMSO/D_2O of complex 7b (red = t_0, green = 48 h)



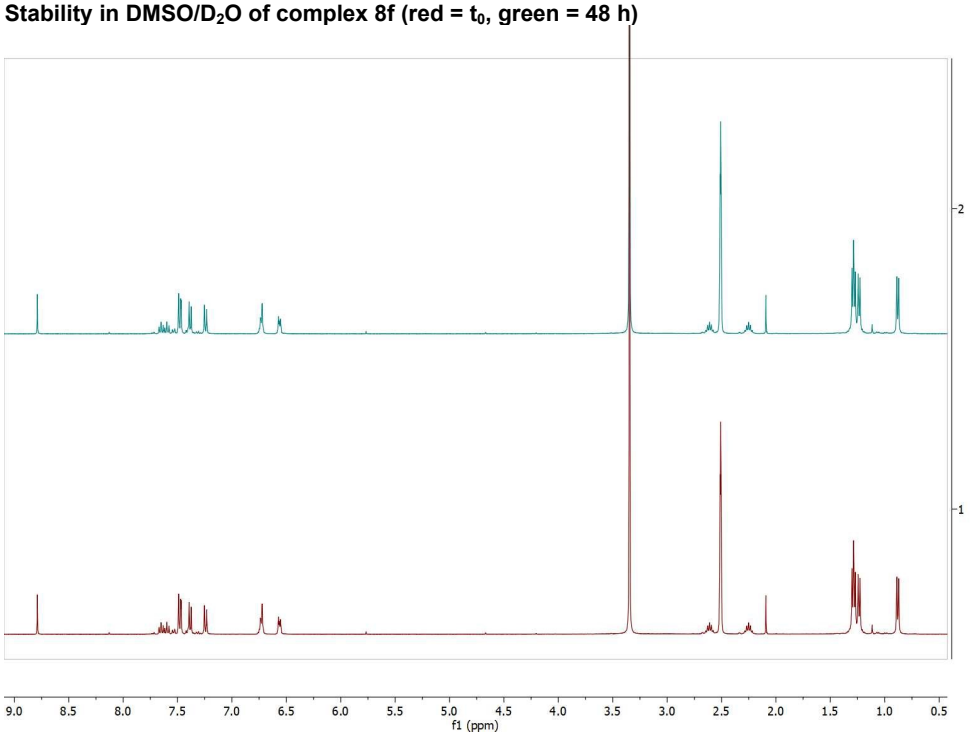
Stability in DMSO/D_2O of complex 7d (red = t_0, green = 48 h)



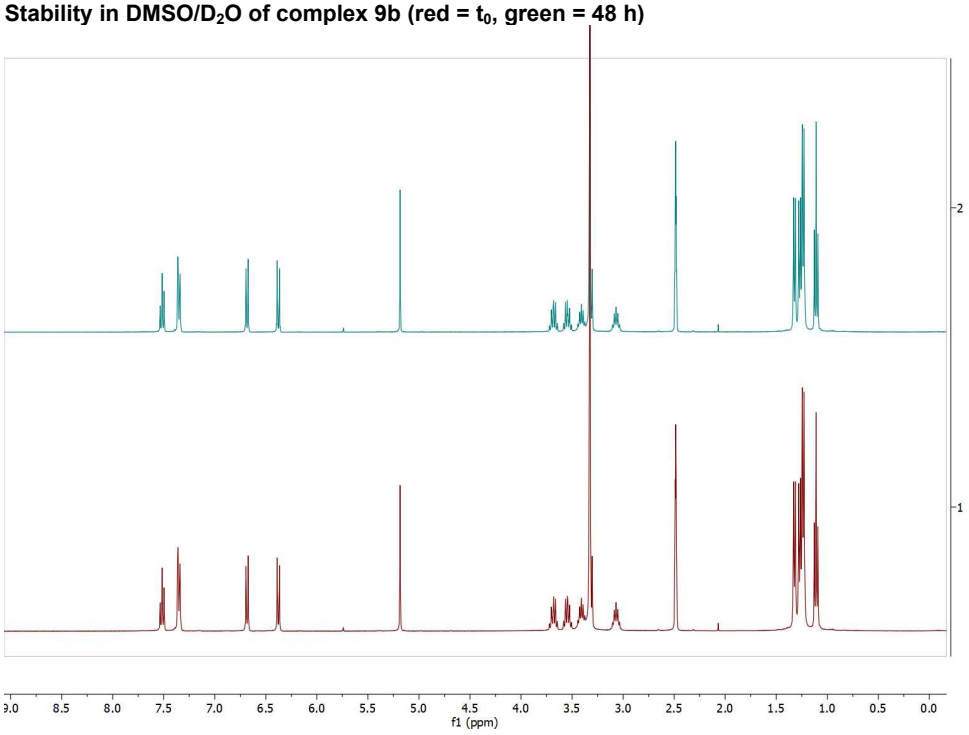
Stability in DMSO/D_2O of complex 8b (red = t_0, green = 48 h)



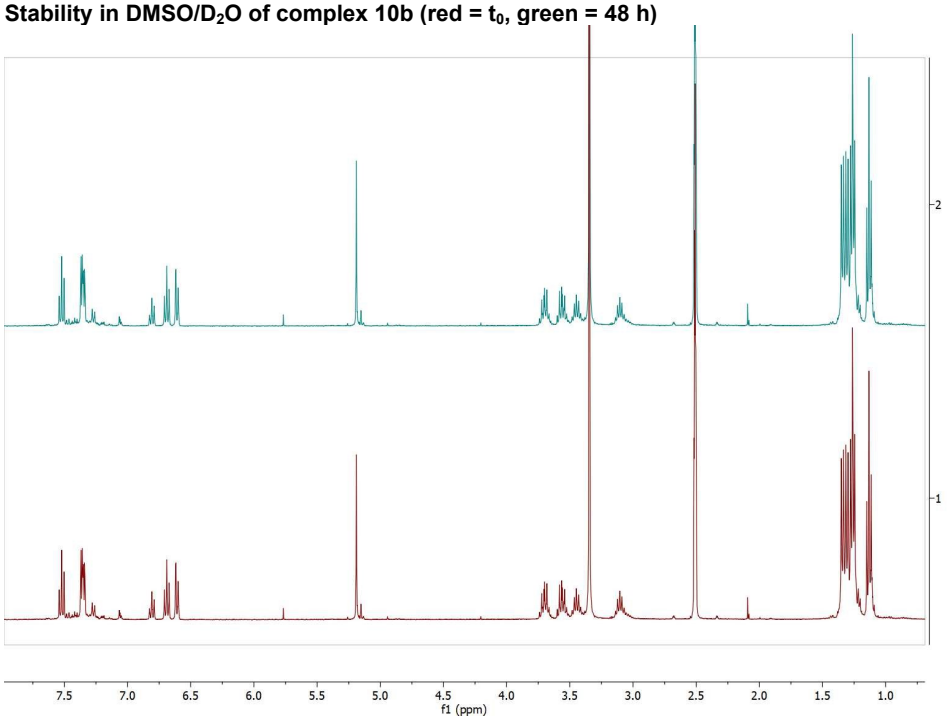
Stability in DMSO/D_2O of complex 8f (red = t_0, green = 48 h)



Stability in DMSO/D_2O of complex 9b (red = t_0, green = 48 h)



Stability in DMSO/D_2O of complex 10b (red = t_0, green = 48 h)



ASA/EDA of [Au(NHC)Cl] complexes

To investigate the electronic properties of NHCs, the gold(I)-chloride complexes bearing backbone ligands **3a-f**, **IPr** and **SIPr** (Figure 1 in the main text) were studied at the ZORA-PBE0/TZ2P-ae//ZORA-BLYP-D3(BJ)/TZ2P level of theory. The ΔE_r values for the reactions of the NHC ligands with gold(I) chloride (AuCl) were inspected according to the Activation Strain Analysis (ASA) approach, also known as distortion-interaction model.[20,21] In this fragment-based method, the energy of the [Au(NHC)Cl] complex (relative to the reactants) is decomposed as the sum of a strain energy (ΔE_{str}) and an interaction energy (ΔE_{int}) (equation 1). The strain term is determined by the extent by which the non-interacting fragments (i.e., the NHC ligand and AuCl) are distorted relative to their equilibrium geometry to reach the structural conformation in the product state. The interaction is instead computed as the energy difference between the products and the separated distorted fragments, and depends on their electronic structure and spatial arrangement. Further insight into the nature of the bond between the fragments was obtained through the Energy Decomposition Analysis (EDA), partitioning the interaction energy into three contributions: the electrostatic interaction (ΔV_{Elstat}), the Pauli repulsion (ΔE_{Pauli}) and the orbital interaction (ΔE_{OI}) (equation 2). ΔV_{Elstat} is the classical coulombian interaction between the unperturbed charge distributions of the fragments (nuclei-nuclei repulsion, nuclei-electron density attraction and electron densities repulsions). ΔE_{Pauli} is a destabilizing contribution arising from the mutual repulsion of same-spin electrons belonging to different fragments. ΔE_{OI} is a term that accounts for charge transfer and polarization effects, resulting from the interaction of occupied orbitals on one fragments and virtual ones in the other.

$$\Delta E = \Delta E_{str} + \Delta E_{int} \quad (1)$$

$$\Delta E_{int} = \Delta V_{Elstat} + \Delta E_{Pauli} + \Delta E_{OI} \quad (2)$$

The reaction energy (ΔE_r) is thus decomposed into strain and interaction contributions (Table S1). [Au(NHC)Cl] are convenient model systems for the study of the bonding properties of NHCs because both the individual reactants and the resulting complex are neutral species, thereby excluding charge delocalization between the fragments. Moreover, the linear coordination geometry of the gold center and the low steric hindrance of the chloride ligand lead to minimal structural distortions upon the formation of the adduct. Consequently, the strain energy contributes marginally to ΔE_r, with values ranging from 0.9 to 2.3 kcal/mol. All reaction energies are substantially negative and increase slightly (become less negative) as the corresponding protonated ligand (NHCH) is associated with a higher coupling constant, which is indicative of a lower σ-donor character. Likewise, the interaction contribution increases slightly with higher ^{1}J(C-H) values. Interestingly, complexes **4a** and **4c** (the only ones bearing 2,4,6-trimethylphenyl substituents on the N atoms) do not follow this pattern, as they exhibit the most stabilizing values of ΔE_r in the entire series, irrespective of their coupling constants. Among the EDA energy terms, only ΔV_{Elstat} values match the expected σ-donor scale: the most negative electrostatic interaction is computed for **4b**, whereas the least negative is found for **4f**. Notably, this correlation is independent of the interatomic distance between the Au center and the NHC carbon, which is nearly identical in all eight cases (1.994-2.000 Å). While orbital interaction contributions do not vary significantly from case to case, ΔE_{Pauli} terms tend to decrease with higher ^{1}J(C-H) values, thereby leveraging the effect of the less stabilizing ΔV_{Elstat}. Although the overall stability of the resulting [Au(NHC)Cl] complexes is marginally influenced by the nature of the NHC ligand, the combination of weaker electrostatic interactions and the lower Pauli repulsion emerging in the presence of backbone substituent such as phenylthioether (**4d**) and phenylsulfonyl (**4f**) suggests that these moieties lead to a diminished electron density on the NHC carbon atom, decreasing its σ-donor strength.

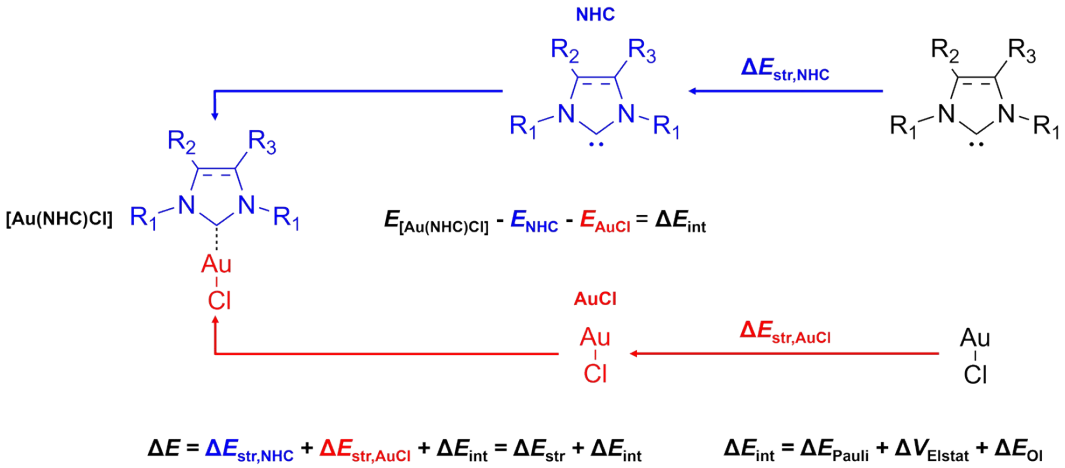


Table S1. Coupling constants of the NHC ligands studied in this work (3) and ASA/EDA energy terms (kcal/mol) relative to their reaction with AuCl, yielding the corresponding [Au(NHC)Cl] complexes (4): reaction energy (ΔE_r), strain energy (ΔE_{str}), interaction energy (ΔE_{int}), Pauli repulsion (ΔE_{Pauli}), orbital interaction (ΔE_{OI}) and electrostatic interaction (ΔV_{Elstat}). Level of theory: ZORA-PBE0/TZ2P-ae//ZORA-BLYP-D3(BJ)/TZ2P.

NHC	^{1}J(C-H) [a] [Hz]	[Au(NHC)Cl]	ΔE_r	ΔE_{str}	ΔE_{int}	ΔE_{Pauli}	ΔE_{OI}	ΔV_{Elstat}
SIPr		**4-SIPr**	-77.9	1.6	-79.5	200.9	-69.2	-211.2
3b	207.3	**4b**	-77.7	2.3	-80.1	204.6	-69.8	-214.9
3a	209.2	**4a**	-78.7	2.1	-80.8	200.0	-68.3	-212.5
IPr		**4-IPr**	-77.9	1.4	-79.4	198.1	-68.4	-209.0
3d	224.7	**4d**	-77.1	1.0	-78.1	196.7	-69.1	-205.6
3e	224.7	**4e**	-76.7	0.9	-77.6	196.5	-69.1	-204.9
3c	225.7	**4c**	-78.1	1.3	-79.4	192.7	-67.5	-204.6
3f	228.1	**4f**	-74.5	1.4	-75.9	196.5	-69.3	-203.1

[a] The ^{1}J(C-H) coupling constant refers to the coupling between NCHN carbon and the proton in the corresponding azolium salt of the ligands (Figure 1 in the main text).

Cartesian Coordinates

Cartesian coordinates (Å), AMS electronic energies (Hartree) and imaginary frequencies (v, cm^{-1}) of all stationary points. Level of theory: ZORA-BLYP-D3(BJ)/TZ2P.

Synthesis of gold(I)-aryl complexes

EtOH
-1.65860624

C	-4.905305640	5.600520590	-4.740416550
H	-4.927816410	6.682838070	-4.925177730
H	-4.112080950	5.170936200	-5.366285790
H	-5.866033220	5.176691350	-5.053371930
C	-4.640026410	5.302712840	-3.263523640
H	-4.613669330	4.221569670	-3.088224630
H	-3.664925150	5.714225520	-2.957316550
O	-5.686823170	5.791565630	-2.392822280
H	-5.734072720	6.758444190	-2.492564640

EtO^-
-1.51143174

C	-4.910757730	5.602485370	-4.730757120
H	-4.948034780	6.688906870	-4.907004760
H	-4.091198120	5.163659410	-5.336771530
H	-5.871319380	5.176720150	-5.060565430
C	-4.711982520	5.324992380	-3.192508840
H	-4.579886290	4.183895590	-3.136856470
H	-3.648698030	5.709213640	-2.981939040
O	-5.667848870	5.828975050	-2.408929340

$PhB(OH)_2$
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B	-3.546708850	8.755156220	-3.248844200
O	-4.900888910	8.921138190	-3.477562750
O	-2.683796440	9.180819100	-4.234281390
H	-5.463791490	8.605447050	-2.753264990
H	-3.157359620	9.558985510	-4.995615220
C	-2.944647830	8.117821580	-1.947070500
C	-3.755846620	7.655488410	-0.891827930
C	-1.547709040	7.990247450	-1.799901300
C	-3.204915200	7.090222580	0.260847240
C	-0.988055830	7.426585450	-0.651240200
C	-1.816058730	6.974964350	0.382521560
H	-4.842015120	7.731743520	-0.957635710
H	-0.900621010	8.339746390	-2.600444380
H	-3.853599340	6.740946530	1.061016430
H	0.092388150	7.338444440	-0.559596330
H	-1.382274690	6.535604900	1.278101310

$[PhB(OH)_2OEt]^-$
-5.20263335

B	-3.564566630	8.700029050	-3.117218180
O	-5.027149340	8.975474090	-2.888970900
O	-2.826594610	9.913057520	-3.546765530
H	-5.077718630	9.792945060	-2.369452020
H	-3.111336490	10.092072760	-4.459163560
C	-2.835315710	8.117550070	-1.755352710
C	-3.559203450	7.492320560	-0.721353400
C	-1.433840170	8.157364810	-1.602342410
C	-2.930401650	6.934839030	0.401661120
C	-0.789660030	7.613126740	-0.484909940
C	-1.537304170	6.993835350	0.527293290
H	-4.644767230	7.452563790	-0.807775580
H	-0.847082460	8.636165960	-2.385049500
H	-3.525321040	6.454787270	1.180624110
H	0.296886410	7.668617830	-0.397744970
H	-1.041214290	6.565885060	1.398537040
O	-3.467771760	7.691573170	-4.225880780
C	-4.191891030	6.489223450	-4.089511980
H	-5.274163320	6.686951740	-3.981314270
H	-3.879251060	5.938721280	-3.179583470
C	-3.950641130	5.604039310	-5.318581280
H	-2.880433510	5.382391170	-5.423722390
H	-4.280625500	6.119934180	-6.230197070
H	-4.500035620	4.654375370	-5.234074450

$EtOB(OH)_2$
-2.64195592

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H	-2.192262140	7.475563880	-1.574286190
H	-2.969687380	10.193721180	-3.450031850
O	-3.932282670	8.078763140	-4.205892950
C	-4.436010670	6.756275340	-4.540637890
H	-5.020484880	6.372270990	-3.694825490
H	-3.586422720	6.079463850	-4.697162160
C	-5.290803650	6.865011220	-5.795359390
H	-4.699794400	7.247506570	-6.635101790
H	-6.137373860	7.540919270	-5.630471370
H	-5.682514340	5.877335860	-6.067445980

4
-11.28883037

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C	0.895763940	8.300534540	1.442569220
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H	2.421411370	10.462056020	-0.701664080
H	0.658057750	8.189891190	2.498102480
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C	-1.699166960	5.401090770	-5.517085970
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C	-2.720958340	5.131958890	-6.437318540
C	-3.966494310	4.673087820	-6.005313690
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H	-2.540331100	5.302450700	-7.496178240
H	-4.751592510	4.473797840	-6.730908070
O	2.352139360	5.412205000	-2.622579690
C	3.456039590	5.659236920	-1.721384580
H	3.515300820	4.867011410	-0.961649480

H	4.357225220	5.642253810	-2.338024350
O	-0.282666540	3.273534990	-2.249287040
C	-0.722363980	2.212364730	-3.128192930
H	0.062209060	1.970164740	-3.859019840
H	-0.904336750	1.347116460	-2.487223950
Au	-2.038008350	8.108685620	-2.540998340
H	-1.643096270	2.482918370	-3.656270910
H	3.362586000	6.632705940	-1.227947160
C	-0.386140050	6.157703610	0.995709900
H	-1.325530620	6.112529670	0.432451760
H	0.122385570	5.196154520	0.851291340
H	-0.625688650	6.251644390	2.058593290
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H	2.432417130	9.644016210	-2.936772200
H	2.094810430	7.923059550	-3.251742780
H	0.778607150	9.097550440	-3.280137540
C	-0.372484820	5.968216560	-5.968556380
H	-0.145064650	6.895387470	-5.429759320
H	0.460171240	5.277125280	-5.786172570
H	-0.394179720	6.188240980	-7.039571790
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TS: 4 + $PhB(OH)_2$ → 5 + $EtOB(OH)_2$ + Cl^-

-16.48561795 v=-207.9

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H	-0.149067890	4.085854290	-4.438577510
H	0.867180590	4.339047840	-1.742707180
C	0.550759780	7.076255330	-1.104913790
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C	1.677121390	9.094974180	-0.438423070
C	0.978687060	7.489907920	1.229250060
C	1.594080230	8.696245250	0.896143890
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C	-2.591165760	5.446636160	-4.469929720
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H	3.133506700	4.623266690	-1.939906890
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O	-0.969608400	3.170922690	-2.769617520
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H	-1.879500110	1.367327130	-3.023247110
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H	2.955928700	6.385209530	-2.190321950
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H	1.384915500	7.929635670	-3.589857660
H	0.260003390	9.224436540	-3.184070830
C	-0.952880010	6.447101610	-6.131046010
H	-0.741384280	7.325458510	-5.508083520
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H	-0.923076470	6.752368330	-7.181693260
Cl	-2.781585890	10.370364840	-3.466402770
H	-5.012884960	8.182078000	-3.318486620
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B	-5.347066530	8.671939230	-1.416777860
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C	-3.496483020	7.315926810	0.354588960
H	-3.968925500	6.407767200	-0.017835130

5

-13.70577267

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N	-0.799965950	5.295632620	-3.203561360
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C	-1.856632600	5.064375410	-4.154462250
C	-3.120748560	4.658801020	-3.686125010

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H	4.455193230	5.551587420	-2.342185880
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H	-1.566933830	2.377335560	-3.640474080
H	3.449421100	6.537132030	-1.237995560
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C	-4.414867650	9.629474340	-3.417360080
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C	-5.047669690	11.853411530	-2.681046230
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H	-6.174040440	10.680072840	-4.102405660
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H	-4.362266920	4.025462310	-2.042450240
H	-2.615493020	3.972424500	-1.692499350
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TS: 4 + EtO^- → 4' + Cl^-

-12.83094285 v=-28.4

C	-0.059878840	4.355679520	-3.818770100
C	-1.267528700	4.389381300	-4.777957260
N	-1.886171750	5.673917830	-4.470951550
C	-1.351329730	6.294123150	-3.364212730
N	-0.300693210	5.503498810	-2.956419250
H	-0.942875960	4.337328610	-5.826243560
H	-0.038053500	3.417208380	-3.247750520
C	0.396216900	5.740012230	-1.723478880
C	1.422035090	6.703648660	-1.680563290
C	-0.009293740	5.028428940	-0.578073700
C	2.105815720	6.878445470	-0.469118770
C	0.705256510	5.226252510	0.611107440
C	1.765106420	6.134377120	0.662165410
H	2.897824980	7.622567530	-0.413171180
H	0.402388920	4.689488410	1.508237400
H	2.305151830	6.286585440	1.594822970
C	-2.987919290	6.229301100	-5.206477890
C	-4.296293670	6.141650600	-4.684433260
C	-2.710577560	6.871780150	-6.428650720
C	-5.337586370	6.677743900	-5.459698060
C	-3.781222350	7.385282960	-7.171894800
C	-5.089125730	7.282416550	-6.692147220
H	-6.354530290	6.625183890	-5.075823550
H	-3.581716470	7.891234600	-8.114819350
H	-5.913982750	7.694020730	-7.271146050
O	1.143222940	4.439174160	-4.608731580
C	2.326483920	4.035548900	-3.899790590
H	2.197459250	3.031233340	-3.465039810
H	3.133805410	4.009402560	-4.637463350
O	-2.083670080	3.237363870	-4.491658430
C	-3.041694470	2.928476530	-5.517846820
H	-2.553474300	2.877567070	-6.504463460
H	-3.454195970	1.946748110	-5.267325570
Au	-2.072574200	7.847515690	-2.415141720
H	-3.849480290	3.667512790	-5.557784310
H	2.583677770	4.737862160	-3.098443970
C	-1.257137850	4.176220400	-0.607585620
H	-2.124037160	4.814566120	-0.824647120
H	-1.227313190	3.399103990	-1.379753450
H	-1.416191660	3.692497900	0.361600870
C	-4.589737760	5.547791190	-3.330808240
H	-5.610106560	5.146064970	-3.305982220
H	-3.886290100	4.749426200	-3.078901370
H	-4.501641140	6.325966310	-2.547802280
C	1.717892240	7.580164380	-2.872235510
H	2.689918220	8.072679390	-2.761010210
H	1.703633620	7.012451500	-3.807930440
H	0.937791260	8.350702550	-2.950082350
C	-1.282418920	7.060592840	-6.888797630
H	-0.680587830	7.498247520	-6.084271260
H	-0.804114320	6.113116440	-7.170533050
H	-1.244912240	7.726442760	-7.757126000
Cl	-1.616591980	10.309590310	-2.103231480
O	-3.855108850	7.783464240	-1.098793280
C	-4.382236590	8.948604430	-0.526285480
H	-4.712090380	9.683449200	-1.291297160
H	-3.633540030	9.485861820	0.089083600
C	-5.591638900	8.596216310	0.364846270
H	-6.372118030	8.101340510	-0.230246630
H	-6.022863050	9.498947180	0.828051900
H	-5.286148600	7.903410750	1.161317870

4'

-12.69213440

C	1.176788820	5.135170670	-1.991887090
C	0.253504260	4.295377500	-2.903122880
N	-0.813139320	5.251760040	-3.253564380
C	-0.697464790	6.437563590	-2.604152370
N	0.426512900	6.395205090	-1.843584480
H	0.792482250	3.973043790	-3.803001180
H	1.304016160	4.645344690	-1.018157200
C	0.819051720	7.448305180	-0.943860930
C	1.518435250	8.559030550	-1.452804940
C	0.474393900	7.332824530	0.415386020
C	1.909686730	9.554301220	-0.546969310
C	0.889694780	8.348048880	1.287580170
C	1.608163490	9.446454170	0.812006880
H	2.449083190	10.423439930	-0.916650460

H	0.630313420	8.281562630	2.341824610
H	1.920094220	10.228927210	1.499892740
C	-1.843497120	4.965493940	-4.217309800
C	-3.110621540	4.553788030	-3.762782240
C	-1.546110920	5.120085280	-5.583789530
C	-4.083061310	4.254127900	-4.726457090
C	-2.545816710	4.804855990	-6.513750480
C	-3.801830560	4.368007560	-6.089162480
H	-5.070767950	3.936647430	-4.400031420
H	-2.339769420	4.921849850	-7.575331620
H	-4.569586440	4.131761470	-6.822289280
O	2.438610210	5.284737160	-2.629475470
C	3.527777130	5.583769540	-1.728165140
H	3.579469270	4.834214490	-0.925442190
H	4.438515480	5.537572980	-2.329391150
O	-0.202100040	3.162201650	-2.176235710
C	-0.630567880	2.057830240	-3.004147490
H	0.162429860	1.778367550	-3.712622750
H	-0.820494260	1.225726450	-2.322580480
Au	-1.934384580	7.972190610	-2.730314320
H	-1.544791220	2.299391910	-3.557369120
H	3.425071960	6.581885080	-1.288121060
C	-0.369515250	6.178872290	0.906773350
H	-1.290830610	6.098148930	0.318256800
H	0.150921400	5.216521300	0.822942760
H	-0.640440580	6.321274100	1.956813670
C	-3.428424440	4.478710290	-2.288059130
H	-4.379496390	3.963833850	-2.123710940
H	-2.641052310	3.962088100	-1.730522080
H	-3.507976680	5.491352350	-1.870966420
C	1.797977670	8.698861210	-2.930399190
H	2.499566640	9.517503030	-3.115451530
H	2.205230700	7.775790400	-3.354422160
H	0.864660590	8.914446300	-3.467517530
C	-0.208304130	5.663984450	-6.030950250
H	0.012280120	6.610254500	-5.523591330
H	0.617193760	4.977256290	-5.804607580
H	-0.207757490	5.841394800	-7.110185320
C	-4.094413160	11.701532330	-2.510335440
H	-5.056916800	11.292128530	-2.180518990
H	-3.921477510	12.655054330	-1.992007910
H	-4.156795410	11.893878860	-3.588249720
C	-2.966257060	10.708385540	-2.213263570
H	-2.001451990	11.149360420	-2.526214640
H	-2.899734440	10.548132010	-1.121373510
O	-3.227812660	9.487288310	-2.903469910

[(4')PhB(OH)$_2$]
-16.33509647

C	0.925631870	5.222477890	-1.818549160
C	0.345497890	4.792023770	-3.187596390
N	-0.863076730	5.637119620	-3.307494800
C	-1.106852200	6.349755370	-2.188869220
N	-0.127134910	6.122390930	-1.290972940
H	1.052085060	5.020903270	-3.994615280
H	1.044758240	4.352004280	-1.161536480
C	-0.096358160	6.728437440	0.015686140
C	0.326291910	8.066837150	0.134864530
C	-0.520894450	5.966404270	1.119182380
C	0.346306290	8.627203140	1.419678530
C	-0.479243900	6.565762440	2.385002690
C	-0.044081090	7.883754550	2.534824800
H	0.666325750	9.659581320	1.540032670
H	-0.807958850	5.998201040	3.252598980
H	-0.022185140	8.337667690	3.522771830
C	-1.656515940	5.762126820	-4.506630340
C	-2.865858400	5.047771050	-4.604789440
C	-1.210352800	6.640392560	-5.510473680
C	-3.624172140	5.212398710	-5.772146790
C	-1.990069570	6.757637780	-6.668569260
C	-3.184942750	6.050138310	-6.799729860
H	-4.569296260	4.683507180	-5.868230870
H	-1.670730290	7.438130130	-7.453323560
H	-3.788560100	6.167293850	-7.696344130
O	2.170954380	5.861922100	-2.028088230
C	3.035278060	5.883763520	-0.868379100
H	3.171937300	4.867126520	-0.473314970
H	3.994365230	6.273257270	-1.215942580
O	0.067950680	3.403109340	-3.151403280
C	-0.020931150	2.782071890	-4.455179440
H	0.889125700	2.982785890	-5.037875690
H	-0.109524240	1.709269270	-4.271758950
Au	-2.687578590	7.509396260	-1.933499640
H	-0.895596140	3.137192820	-5.010755660
H	2.634878140	6.532037910	-0.081537250
C	-1.055891300	4.564169510	0.937897950
H	-1.833334220	4.540536740	0.165664870
H	-0.273654490	3.859037830	0.628821820
H	-1.485399390	4.193645890	1.872916690
C	-3.363583000	4.177531280	-3.474415160
H	-4.173170070	3.526746550	-3.816735650
H	-2.563856210	3.561686910	-3.052065830
H	-3.750961620	4.804897870	-2.660435320
C	0.707305360	8.888344320	-1.074386990
H	1.225868450	9.802028370	-0.769990640
H	1.350144630	8.327460830	-1.759339270
H	-0.187089600	9.181201790	-1.639240410
C	0.013472420	7.501158080	-5.307494130
H	-0.166655200	8.225307700	-4.504258830
H	0.901417520	6.919667160	-5.036057670
H	0.238999620	8.067481580	-6.214021550
H	-4.403902440	9.053136980	0.936520600
C	-4.863510630	8.122283230	0.585363130
H	-5.670301360	7.847971270	1.277310360
H	-4.101395340	7.332547390	0.615857840
H	-6.172063660	9.090996600	-0.852072060
C	-5.418038240	8.297074170	-0.825034920
H	-5.882656060	7.367860090	-1.185899530
O	-4.373664710	8.704544750	-1.739075150
B	-4.859076240	9.245592440	-3.253004800
O	-5.884080390	10.227436470	-3.013895390
H	-6.734979840	9.874650090	-3.320174400
O	-5.393591640	8.106425290	-3.982060650
H	-4.695998870	7.525295740	-4.322360320
H	-2.842958070	10.780255340	-1.971845270
C	-2.596624950	10.636999320	-3.021577740
C	-3.471855020	9.876921740	-3.826453820
H	-3.781551250	9.169290940	-5.838307480
C	-1.429897920	11.211417810	-3.537045180
H	-0.775702050	11.792391680	-2.888483530
C	-1.107985680	11.051851250	-4.890092810
H	-0.204810760	11.501933500	-5.297899750
C	-1.966280370	10.315926690	-5.713541470
H	-1.731171210	10.193836430	-6.769986340
C	-3.124190190	9.737498010	-5.183049000

TS: [(4')PhB(OH)$_2$] → 5 + EtOB(OH)$_2$

-16.31117941 v=-114.9

C	0.408050300	4.763339430	-3.443834070
C	-0.544474230	4.403032700	-4.610422110
N	-1.578015740	5.461979190	-4.523452760
C	-1.398740050	6.273004500	-3.461580130
N	-0.280312370	5.907239340	-2.804320660
H	-0.016701150	4.464308840	-5.570777710
H	0.483126560	3.924952920	-2.739265930
C	0.107912360	6.486012400	-1.541514350
C	0.893429090	7.653010680	-1.541184030
C	-0.361966060	5.887843560	-0.357830790
C	1.259664520	8.190592680	-0.299905610
C	0.032661370	6.455319490	0.861323870
C	0.844424660	7.590631660	0.890452770
H	1.864347400	9.094137350	-0.271851260
H	-0.318990160	6.012659800	1.790377090
H	1.138182880	8.021419030	1.844845040
C	-2.681758920	5.604571070	-5.440126430
C	-3.945706930	5.103935450	-5.068210790
C	-2.462547000	6.283600330	-6.652379340
C	-5.005777270	5.289990590	-5.967657280
C	-3.548185310	6.435883200	-7.524906120
C	-4.809320750	5.942930280	-7.185445680
H	-5.995200870	4.930458290	-5.696814490
H	-3.404479980	6.964955490	-8.464234740
H	-5.646525150	6.082260000	-7.865038450
O	1.684898300	5.080362240	-3.969159730
C	2.768592010	4.933169730	-3.022547280
H	2.768858280	3.920680880	-2.594863410
H	3.687866230	5.090829110	-3.590516410
O	-1.044014950	3.095040660	-4.402395090
C	-1.548197130	2.449654680	-5.594771630
H	-0.787689060	2.463752330	-6.388371740
H	-1.761339280	1.417226030	-5.310072200
Au	-2.657555330	7.721973470	-2.870990410
H	-2.463407560	2.931429300	-5.954911060
H	2.700369510	5.670487300	-2.215093660
C	-1.335188240	4.732796400	-0.401318080
H	-2.286599640	5.061122440	-0.837179430
H	-0.972402520	3.895647520	-1.008307570
H	-1.537166640	4.359993120	0.606535110
C	-4.178461680	4.442587180	-3.731230430
H	-5.113842050	3.875910080	-3.742600850
H	-3.357934900	3.771580670	-3.462403330
H	-4.258683250	5.204225220	-2.944414810
C	1.268806090	8.343889100	-2.831122440
H	2.018975730	9.119191480	-2.650400650
H	1.654007240	7.640593980	-3.575413330
H	0.381358470	8.820778860	-3.268315070
C	-1.112346970	6.881642860	-6.976359820
H	-0.767202430	7.527512480	-6.160632410
H	-0.343895430	6.112417360	-7.125810640
H	-1.166632070	7.479188620	-7.890717700
H	-4.777645370	5.511542560	0.745943790
C	-5.341989400	5.048334770	-0.072400930
H	-6.092678730	4.374100920	0.359870130
H	-4.645366100	4.447230450	-0.669153190
H	-6.735904800	6.692609240	-0.329605570
C	-6.012293990	6.122248450	-0.927697290
H	-6.571461460	5.654451150	-1.756638880
O	-5.007216130	7.003815440	-1.443746810
B	-5.468262650	8.166488830	-2.220016180
O	-6.506452900	8.902406200	-1.543702050
H	-7.080601860	9.324762130	-2.202006380
O	-5.852917610	7.925700460	-3.606028980
H	-5.211540380	7.366130620	-4.070906870
H	-3.531053310	8.876571310	-0.102411430
C	-3.485617910	9.634549180	-0.881213240
C	-3.993583660	9.301561040	-2.169686930
H	-4.340029140	10.106404650	-4.144349320
C	-2.976030830	10.899974350	-0.593789460
H	-2.602924450	11.129917070	0.402712870
C	-2.950686840	11.882827100	-1.592716840
H	-2.560802360	12.874181310	-1.369070970
C	-3.428963480	11.593867760	-2.876794260
H	-3.407740860	12.361058090	-3.648994920
C	-3.936640880	10.323942720	-3.157408020

<u>Synthesis of gold(I)-selenolato complexes</u>

5-Se

-13.76756133

C	1.295579720	5.177946760	-2.246148780
C	0.078388310	4.270281730	-2.543200120
N	-1.042336340	5.233477400	-2.567823540
C	-0.660093280	6.497919850	-2.287905280
N	0.670029620	6.506340130	-2.054497180
H	0.188741900	3.794083670	-3.526623060
H	1.802824600	4.854471820	-1.328404810
C	1.407329740	7.689634290	-1.694113680
C	1.750000900	8.616986350	-2.697981650
C	1.746711070	7.881482240	-0.341909810
C	2.479919960	9.750479160	-2.312627530
C	2.481955320	9.025211230	-0.003378580
C	2.850216300	9.950431680	-0.981791040
H	2.754419020	10.482410510	-3.068766310
H	2.750349370	9.195594810	1.036892990
H	3.416902810	10.836241420	-0.704170630
C	-2.380727410	4.901995800	-2.992558160
C	-3.339704910	4.584635440	-2.012327580
C	-2.691133460	4.959371060	-4.363601710
C	-4.632256300	4.259621640	-2.443925390
C	-3.995890390	4.622733660	-4.751887500
C	-4.954804280	4.266319440	-3.803016030
H	-5.391527430	4.012834510	-1.705213880
H	-4.260986320	4.663816170	-5.805762040
H	-5.962932350	4.010938060	-4.121495060
O	2.186782040	5.119420770	-3.347927840
C	3.546675600	5.500232680	-3.039015640
H	3.926379070	4.912876000	-2.190702490
H	4.132870080	5.273001400	-3.932076560
O	-0.023220710	3.281416830	-1.531076820
C	-0.736352760	2.090903650	-1.936591380
H	-0.286368900	1.664713200	-2.844432560
H	-0.634780710	1.382795430	-1.111289590
H	-1.796715150	2.298589150	-2.118394430
H	3.622678240	6.568228240	-2.807978660
C	1.293311610	6.906708300	0.721398190
H	0.222701950	6.694165240	0.625471570
H	1.820891480	5.946327200	0.653075210
H	1.478349210	7.314645510	1.719271690
C	-3.006802030	4.667918460	-0.540952220
H	-3.819884390	4.255057910	0.063386640
H	-2.079127580	4.140617030	-0.299679540
H	-2.862758290	5.718068340	-0.253084590

C	1.325368110	8.425923080	-4.134828680
H	1.892818540	9.089276350	-4.794179750
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C	-1.694591640	5.472153100	-5.376289660
H	-1.640217890	6.567742550	-5.307479210
H	-0.684622570	5.082189570	-5.215406060
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Au	-1.907520550	8.097611210	-2.441340390
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H	-4.791128010	8.380899810	-3.621102710
C	-3.003674810	11.009767330	-2.306062890
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TS-5-10

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C	2.399853880	9.788446210	-2.367035340
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H	2.673944690	10.513045370	-3.130389830
H	2.622365240	9.292136240	0.995261510
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C	-3.353015170	4.545169460	-2.040309940
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C	-3.975381160	4.519713590	-4.788169110
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H	-5.398722230	3.944266550	-1.747379820
H	-4.227902750	4.535493940	-5.845856710
H	-5.939383370	3.885705330	-4.170023550
O	2.172976920	5.127222130	-3.348978390
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H	4.117383500	5.298328700	-3.933398720
O	-0.020134780	3.298623870	-1.501769380
C	-0.716324980	2.091701900	-1.887028180
H	-0.257044230	1.653514870	-2.784474420
H	-0.609783800	1.400943400	-1.047723370
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H	0.136523360	6.763946190	0.591679610
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H	-2.905173960	5.715757260	-0.298011690
C	1.299410250	8.419316720	-4.187786700
H	1.910882540	9.039083140	-4.850575720
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H	-1.612031820	6.488630030	-5.326785830
H	-0.672410420	4.992997470	-5.237372910
H	-1.991509720	5.141496340	-6.416330750
Au	-1.936196690	8.077731330	-2.462917270
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H	-4.827722370	8.485332280	-3.600902480
C	-2.923409220	11.009844130	-2.254049550
H	-1.900016570	11.235593610	-1.965629440
C	-3.911352990	11.950381690	-2.087875510
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C	-0.433018690	6.349989550	-5.837756510
C	-2.983032080	5.222361640	-6.224708410
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O	2.393683070	5.443113430	-1.857948220
C	3.101571510	5.409107470	-0.597742910
H	3.016222530	4.414872650	-0.136371560
H	4.147962090	5.613411290	-0.834551650
O	0.064226550	3.263755890	-3.099146710
C	0.057717120	2.551425750	-4.357238570
H	1.058230680	2.567557270	-4.812528010
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H	-0.668861330	2.977672620	-5.057582390

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H	-2.141225020	5.001232460	-0.267487750
H	-0.817042710	4.015274260	0.353390090
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H	-4.006681180	3.957843250	-4.150774430
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C	-2.913262760	2.827870660	0.709255380
H	-3.767160950	2.656392180	0.042456830
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C	3.042476690	6.281358570	2.026121680
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H	-1.038505380	8.047690960	-6.536634490
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C	-2.403168970	4.741356690	-2.145100920
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C	-2.370268580	4.705071020	-2.173849740
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H	0.761161440	1.854587710	-1.562304080
H	0.719668180	2.138211710	0.188762000
C	-1.239176970	1.840693070	-0.698642230
H	-1.769252920	2.015643300	-1.639411600
H	-1.238481990	0.761193430	-0.499335740
H	-1.796108180	2.343775210	0.097780630
C	4.008614980	6.017879900	-4.113052950
H	3.915042280	6.600879120	-3.192167740
H	5.071440040	5.794273900	-4.272478930
H	3.653287610	6.639969870	-4.940259300
H	0.584654770	8.482116680	-6.059697520
H	-0.598870080	7.901593370	-4.858355950
H	2.579466850	8.231581230	0.375474830
H	1.226745900	7.183284470	-0.114737450
H	-3.028012330	5.745781230	1.040612390
H	-2.186469480	6.747419400	-0.171585920
H	-1.701031570	4.652332470	-4.831742340
H	-2.981389730	3.516626480	-5.321666000
C	-6.347107410	3.107476980	-1.614066410
H	-6.570676550	2.315441670	-2.336745520
H	-6.477508890	2.698700950	-0.604994580
H	-7.098537900	3.898478440	-1.744148470
C	3.748448360	11.314580020	-3.415625560
H	4.581700880	11.377728930	-2.707465970
H	4.157224170	11.353390700	-4.432127360
H	3.128455160	12.211499480	-3.279199910

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-16.88101368

C	1.268233900	5.242994080	-2.658407760
C	0.113830570	4.313577640	-2.215382710
N	-1.051898720	5.221329210	-2.314653420
C	-0.742333410	6.529902040	-2.496719440
N	0.606828460	6.567781600	-2.636240440
H	0.022057430	3.465049140	-2.901082410
H	2.094298820	5.194367290	-1.941575780
C	1.371050920	7.765330140	-2.844176560
C	1.414894470	8.348807980	-4.126207480

C	2.088325850	8.298668090	-1.750743340
C	2.216222340	9.487729320	-4.298200850
C	2.887001310	9.427349420	-1.974611800
C	2.954338510	10.014591780	-3.239866870
H	2.266168650	9.965129600	-5.273095850
H	3.452296210	9.861150320	-1.155158350
H	3.577792660	10.892296700	-3.396807800
C	1.909857310	7.716238080	-0.350483750
H	1.697173380	6.647117930	-0.449077190
C	0.575060580	7.809971360	-5.278653740
H	0.268211010	6.795993590	-5.015082450
C	3.153680570	7.851051350	0.547387080
H	4.045411350	7.434788850	0.064009470
H	3.363210570	8.896786930	0.801163410
H	2.991875900	7.313672240	1.488960920
C	0.665840320	8.353386350	0.315491860
H	0.478632400	7.896820070	1.295226560
H	0.819333710	9.430043080	0.458562630
H	-0.220546850	8.213084250	-0.309585210
C	1.354665070	7.716750860	-6.605363110
H	0.727217920	7.247916210	-7.372672180
H	1.650333920	8.703474730	-6.980966810
H	2.260113660	7.110679930	-6.490510260
C	-0.705213820	8.663193940	-5.436701330
H	-1.335029400	8.263431420	-6.240648230
H	-1.281252130	8.654981990	-4.506245360
H	-0.452219680	9.702222310	-5.682516360
C	-2.383271760	4.717820340	-2.126793840
C	-3.004261020	4.845644260	-0.868302780
C	-3.013600490	4.073001760	-3.213767710
C	-4.284514390	4.292898530	-0.712518550
C	-4.284955670	3.523239330	-3.005933120
C	-4.913747420	3.627999730	-1.763378220
H	-4.792836660	4.380642490	0.243905260
H	-4.796293000	3.019480790	-3.820770540
H	-5.902343900	3.197281750	-1.618911250
C	-2.346761810	5.611820480	0.273913240
H	-1.285420550	5.707514940	0.037210140
C	-2.362928660	4.071708040	-4.595192790
H	-1.276544690	4.066794580	-4.461728090
C	-2.940590170	7.037371250	0.357942120
H	-2.450467640	7.610154460	1.154482120
H	-2.793667100	7.563565920	-0.590304660
H	-4.015733340	6.998867700	0.573816450
C	-2.444482120	4.881933300	1.628313690
H	-1.887507840	5.438600100	2.391352870
H	-3.480424300	4.794277270	1.976521300
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C	-2.711081460	5.390504530	-5.327726400
H	-2.412558790	6.255150520	-4.728294970
H	-2.195262960	5.440417600	-6.294597650
H	-3.791358620	5.452795020	-5.507654060
C	-2.720434490	2.845233160	-5.455036890
H	-2.131256550	2.855422460	-6.379318050
H	-2.511294000	1.908191160	-4.925571570
H	-3.778184020	2.842503310	-5.743193930
O	1.727028970	4.917482330	-3.971536670
C	3.145033500	4.628106590	-4.071470830
H	3.422159250	3.890618650	-3.301757010
H	3.253180190	4.147677380	-5.049377780
O	0.297229130	3.854533090	-0.875068720
C	0.297060190	2.412670040	-0.715565820
H	0.990313050	1.964737110	-1.444873890
H	0.713883190	2.252560720	0.284133970
C	-1.091676610	1.784116730	-0.829652540
H	-1.525829710	1.931831690	-1.823577580
H	-1.020378410	0.704631860	-0.644991440
H	-1.777444080	2.221933840	-0.099090900
C	4.031690930	5.869753970	-3.977825000
H	3.939842250	6.364213010	-3.005545800
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H	3.762701180	6.598126130	-4.747758620

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-12.88396512

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C	-1.599603060	6.924411870	-1.612447140
N	-2.891736730	6.885455650	-2.200193320
C	-2.867102580	7.057467500	-3.563040720
N	-1.514585410	7.170851470	-3.810579460
H	0.341246390	7.201643920	-2.659410700
C	-0.966854980	7.362695620	-5.129469620
C	-0.581740100	6.238299910	-5.875875950
C	-0.842976930	8.668707910	-5.629899680
C	-0.044977700	6.450004250	-7.152563050
C	-0.302082420	8.832315170	-6.911307060
C	0.107093260	7.737197780	-7.684036940
H	0.252379870	5.587606360	-7.747065250
H	-0.205311170	9.838458700	-7.316361970
C	-1.306039080	9.854769280	-4.814851570
H	-2.373372640	9.767511800	-4.581032470
C	-0.772152460	4.843615200	-5.324580210
H	-0.212609020	4.699937940	-4.392041950
C	-4.104905510	6.800688240	-1.428255130
C	-4.836526110	7.978163770	-1.190933150
C	-4.500002630	5.561582000	-0.904661530
C	-5.957663460	7.896899070	-0.360399540
C	-5.629515740	5.530671970	-0.074279830
C	-6.358542900	6.687376870	0.222159900
H	-6.523525190	8.803694770	-0.153641030
H	-5.946190370	4.576879200	0.344807890
C	-4.434604090	9.287274790	-1.826552470
H	-3.373067240	9.498842350	-1.667243040
C	-3.740998740	4.296217840	-1.231178450
H	-2.776644040	4.269615770	-0.709518220
S	-1.214811290	6.581177420	0.069882780
C	-2.196975960	7.817099480	0.943088800
C	-3.124363120	7.382064470	1.897902580
C	-2.026428800	9.185530790	0.698191900
C	-3.887400820	8.318095130	2.599462830
C	-2.804670410	10.114788230	1.391115280
C	-3.735918290	9.684141540	2.343103370
H	-3.270379730	6.318431450	2.058922840
H	-1.298715480	9.513211050	-0.039212940
H	-4.617217950	7.976607100	3.329529900
H	-2.681549750	11.176417630	1.189635710
H	-4.341438780	10.410499860	2.879605230
H	-0.437659670	4.092198780	-6.045837480
H	-3.532943320	4.233395070	-2.305002890
H	-0.775271820	9.913451770	-3.856454970
H	-5.017798730	10.113399660	-1.409223430
H	-4.592644460	9.247214540	-2.910720390
H	-4.316256570	3.414525620	-0.932660010
H	-1.828408240	4.663421790	-5.091684460
H	-1.138488890	10.788890930	-5.358996700
C	0.718829000	7.942978290	-9.053577790

H	1.803818560	8.100229090	-8.977270150
H	0.557384040	7.071454920	-9.697259490
H	0.294820440	8.822182650	-9.551358920
C	-7.544433550	6.645216720	1.161401770
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H	-7.846563500	5.615386050	1.378347000
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-16.38185826

C	-0.976402840	6.886719270	-2.457089260
C	-1.896506710	6.698572440	-1.465258440
N	-3.152927390	6.653335590	-2.123304780
C	-3.053533860	6.805790940	-3.482787720
N	-1.687188930	6.949045390	-3.651725270
H	0.097325600	6.983286820	-2.401745020
C	-1.074047770	7.287342170	-4.912822530
C	-0.642844410	6.252090360	-5.763438980
C	-0.925173240	8.650816660	-5.231065230
C	-0.026680440	6.619729730	-6.967828630
C	-0.295953050	8.968249290	-6.443381420
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H	0.315918040	5.849978100	-7.653177980
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H	0.635766650	8.228270550	-8.238652680
C	-1.417448480	9.750951980	-4.294176160
H	-2.040413880	9.281797940	-3.528642630
C	-0.910917160	4.791199190	-5.418227630
H	-1.025114370	4.723452220	-4.330924920
C	-0.234574280	10.440687170	-3.577119450
H	0.371616990	9.713536560	-3.025279730
H	0.421121300	10.945434800	-4.296818850
H	-0.602058070	11.191309370	-2.866652350
C	-2.308216360	10.778923200	-5.022250010
H	-2.706996830	11.504783220	-4.303810580
H	-1.748488270	11.335726430	-5.782706080
H	-3.151934270	10.282289200	-5.511774550
C	0.237101160	3.845426510	-5.821008630
H	0.032219040	2.833845220	-5.451714900
H	0.348231940	3.778632750	-6.909591820
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H	-2.199647370	4.405360550	-7.141981270
C	-4.406889620	6.468546170	-1.431711810
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C	-4.789979600	5.160369430	-1.080258070
C	-6.401289450	7.387803320	-0.461800480
C	-6.010196560	4.999456970	-0.411006970
C	-6.808929480	6.102525740	-0.106153260
H	-7.032821040	8.235928050	-0.214862200
H	-6.341450320	4.005157660	-0.126715510
H	-7.754056930	5.958928130	0.413197850
C	-4.756550470	8.999754910	-1.556353310
H	-3.666524320	8.992496560	-1.652345570
C	-3.938038530	3.960001930	-1.479951130
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C	-5.341568060	9.337808200	-2.948424940
H	-5.011775340	10.334132120	-3.267635420
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C	-5.111447480	10.083812370	-0.521680510
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H	-4.740172230	9.821740750	0.473050800
C	-4.371118400	3.453151620	-2.876728500
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H	-3.725131260	2.628819410	-3.203473300
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C	-3.950908180	2.824626680	-0.439246620
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H	-3.674362030	3.195520460	0.553939140
H	-4.935635730	2.348436060	-0.365422810
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C	-1.538670940	9.340952780	0.108284350
C	-2.718328240	9.669178160	2.623249080
C	-1.725636900	10.620052500	0.634676680
C	-2.307868600	10.790447570	1.895812300
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-16.32294314

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C	-1.873134000	6.693022540	-1.467411840
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N	-1.676918150	6.946255590	-3.654185250
H	0.116257470	6.968205700	-2.416579770
C	-1.071049170	7.286697820	-4.918582090
C	-0.652642130	6.252905080	-5.777218570
C	-0.916734210	8.650928880	-5.231036720
C	-0.042766070	6.622964340	-6.984070020
C	-0.294028760	8.970560100	-6.446104610
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H	0.290232680	5.854698530	-7.675733370
H	-0.153368180	10.012915660	-6.719678000
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C	-0.927985520	4.792104970	-5.437359360
H	-1.030187280	4.718793980	-4.349148330
C	-0.205362440	10.421061070	-3.564562140
H	0.393750360	9.683773910	-3.018328280
H	0.455265460	10.923173380	-4.281493030
H	-0.563679900	11.171905180	-2.849534760
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H	-1.712415320	11.351009490	-5.758711980
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H	-0.000871460	2.827746400	-5.492547560
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C	-2.281527420	4.363161770	-6.053973580
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H	-2.239162520	4.426439910	-7.148394120
C	-4.384841650	6.476739060	-1.415711860
C	-5.163501190	7.610028750	-1.115086350

C	-4.764889580	5.170153280	-1.054371460
C	-6.372421580	7.400268410	-0.435573580
C	-5.979129060	5.012599710	-0.373531890
C	-6.775660910	6.116997000	-0.067984620
H	-7.002759560	8.249238480	-0.188835720
H	-6.307676130	4.019785250	-0.081219300
H	-7.716082820	5.976041330	0.460480100
C	-4.741036840	9.007792540	-1.555111500
H	-3.650099510	9.006768290	-1.644070390
C	-3.918065900	3.967291020	-1.457791190
H	-2.881018120	4.305444880	-1.550958730
C	-5.319246060	9.327281610	-2.954623000
H	-4.995842450	10.323492320	-3.280507490
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H	-6.415839620	9.314841440	-2.925628850
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H	-6.196599470	10.268234340	-0.499460370
H	-4.770334830	9.846309270	0.468849380
C	-4.359626560	3.461956970	-2.852584890
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H	-3.647351540	3.200815580	0.574638590
H	-4.914553390	2.357421760	-0.339921340
S	-1.625671530	6.522720720	0.260419280
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C	-2.598666170	8.360454110	2.068471840
C	-1.538399640	9.328045540	0.116085890
C	-2.813730840	9.638959550	2.589809080
C	-1.767227480	10.607414890	0.620704790
C	-2.399729550	10.752969910	1.857976820
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H	-1.043579390	9.210248850	-0.842683450
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-16.76903597

C	-0.846115200	7.134880420	-2.652187170
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-17.13996367

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C	-2.178776750	5.402866540	0.464315210
H	-1.168972250	5.637138970	0.119475060
C	-2.594892360	4.403947950	-4.546011190
H	-1.528091320	4.639280610	-4.481731200
C	-2.835130940	6.725016650	0.923710450
H	-2.242665630	7.184340630	1.723894400
H	-2.903045870	7.435367340	0.093138370
H	-3.848182080	6.550758160	1.305458680
C	-2.038395430	4.407929430	1.635189190
H	-1.457523400	4.862935920	2.446232170
H	-3.015227910	4.124695060	2.044320910
H	-1.521817510	3.496853260	1.316728490
C	-3.263412820	5.573683560	-5.305881770
H	-3.129615900	6.515185380	-4.762801520
H	-2.823091340	5.681902480	-6.304335890
H	-4.339537780	5.398303980	-5.420189800
C	-2.724520840	3.076031010	-5.320622950
H	-2.247659450	3.165036730	-6.303641720
H	-2.245772610	2.250234470	-4.780945410
H	-3.773620940	2.805263470	-5.484658080
O	1.938360800	4.899303660	-3.783519530
C	3.375887080	4.703975630	-3.649639570
H	3.567899680	4.032214930	-2.799740280
H	3.653977430	4.175585700	-4.566585660
O	0.280278150	3.637044920	-1.057351330
C	0.189528490	2.184912120	-1.132117890
H	0.838374810	1.827456620	-1.945567570
H	0.620024810	1.847509870	-0.184414620
C	-1.235023640	1.660787920	-1.299767280
H	-1.678050950	1.976890900	-2.248937470
H	-1.219648910	0.563755060	-1.281107230
H	-1.882040630	2.016881840	-0.493717800
C	4.167062350	6.002558310	-3.508667660
H	3.911781620	6.539409100	-2.590106220
H	5.238991520	5.769821400	-3.478980260
H	3.976149370	6.672205990	-4.351445300
Au	-2.001246110	8.065357760	-2.552733350
Cl	-3.468983990	9.852273910	-2.617119110

C	-6.380646450	6.657969510	0.169478080
H	-6.525284370	8.786526130	-0.130163940
H	-5.973156630	4.542382630	0.240712430
C	-4.396803900	9.323722040	-1.727020810
H	-3.313515290	9.467208000	-1.690222650
C	-3.723631010	4.310800410	-1.288435060
H	-2.727209280	4.306563290	-0.830962770
S	-1.178213690	6.622211740	0.101838200
C	-2.172361770	7.852934730	0.971750260
C	-3.131588760	7.407897900	1.888811730
C	-1.972765770	9.222705030	0.761376460
C	-3.900970120	8.339650850	2.589036360
C	-2.757692360	10.147472300	1.452988460
C	-3.721415110	9.708353020	2.367845480
H	-3.297125530	6.343300050	2.021166480
H	-1.218084350	9.556752910	0.054681460
H	-4.656638050	7.993237400	3.289462920
H	-2.613442460	11.211300120	1.280281540
H	-4.330962510	10.431489740	2.903933060
H	-0.453551490	4.081366710	-6.013662650
H	-3.589032180	4.239109520	-2.374141100
H	-0.790383520	9.882748860	-3.825608340
H	-4.871980520	10.146061400	-1.185354810
H	-4.697862380	9.378078660	-2.781220020
H	-4.260562290	3.420884360	-0.948093350
H	-1.909246120	4.661901300	-5.177984120
H	-1.024712440	10.794350320	-5.331822390
C	0.605600460	7.903137830	-9.099658460
H	1.685735580	8.101490150	-9.062177510
H	0.453857570	7.010873050	-9.715857920
H	0.133211930	8.754082440	-9.602616340
C	-7.634525080	6.571993880	1.011720700
H	-8.525448120	6.492188460	0.374109180
H	-7.617314230	5.693998990	1.666232640
H	-7.757171350	7.465790280	1.633803900
Au	-4.307577170	7.106729330	-4.805598750
Cl	-6.055619180	7.170935640	-6.315983200
H	0.380863730	7.222767520	-2.638802500

4c

-13.13746940

C	-0.694344490	7.137515460	-2.624644540
C	-1.558634330	6.960342300	-1.578834400
N	-2.852770460	6.914373950	-2.148712520
C	-2.795401270	7.062691920	-3.507112710
N	-1.459823470	7.184782750	-3.787787640
C	-0.934984870	7.364693460	-5.121756070
C	-0.605717390	6.227571190	-5.873516880
C	-0.814110570	8.668775570	-5.626302530
C	-0.110032490	6.427780130	-7.167620730
C	-0.314766220	8.816932820	-6.924861720
C	0.047297120	7.711096470	-7.706499890
H	0.143080870	5.559074500	-7.772392360
H	-0.222050100	9.818805860	-7.340079620
C	-1.263920560	9.861256140	-4.814379650
H	-2.348632800	9.823601290	-4.653546380
C	-0.836074670	4.838953760	-5.324188990
H	-0.349504550	4.698880460	-4.351649970
C	-4.081178150	6.820327440	-1.396336840
C	-4.808084050	7.994643960	-1.142395040
C	-4.488238370	5.562791860	-0.928074530
C	-5.955516430	7.886014780	-0.350726720
C	-5.641410040	5.508072510	-0.136476880

4d

-16.63767911

C	-1.002016190	6.930741510	-2.405895510
C	-1.955957390	6.767000070	-1.438769310
N	-3.198725220	6.785228320	-2.114579060
C	-3.022584920	6.938593380	-3.459180780
N	-1.662568310	7.038731500	-3.620734930
H	0.072628870	6.980381580	-2.327024010
C	-1.023864510	7.280872380	-4.894919370
C	-0.630377320	6.175826980	-5.669629790
C	-0.860187120	8.616243100	-5.306088230
C	-0.019845750	6.446229230	-6.902158840
C	-0.244166780	8.831666180	-6.546094470
C	0.175776390	7.758582780	-7.332817060
H	0.291557210	5.621349340	-7.537040990
H	-0.105654970	9.847534910	-6.905972730
H	0.646169290	7.946427620	-8.295177010
C	-1.385549600	9.787345620	-4.481910340
H	-1.746608960	9.396276870	-3.525753520
C	-0.908961990	4.741440240	-5.234161240
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C	-0.281698240	10.818298950	-4.164318110
H	0.561463100	10.349104960	-3.643861830
H	0.105109690	11.286552640	-5.076577200

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H	-3.379340550	9.702278740	-5.377519600
C	0.371547080	3.879716380	-5.218446540
H	0.144755110	2.874439650	-4.844553070
H	0.795767130	3.773061770	-6.223420640
H	1.139966330	4.321822830	-4.573541220
C	-2.008809800	4.113619330	-6.121019190
H	-2.252730900	3.105399290	-5.766416630
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H	-1.676824370	4.039741560	-7.163184680
C	-4.488131510	6.546143690	-1.502900410
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C	-4.905734140	5.210404530	-1.364146370
C	-6.524956140	7.368913430	-0.549945440
C	-6.166756450	4.987699390	-0.796437730
C	-6.967607310	6.055794170	-0.392769610
H	-7.165885650	8.190018210	-0.242604740
H	-6.529800620	3.970225530	-0.680735940
H	-7.947199640	5.863995980	0.039129430
C	-4.822017410	9.086110260	-1.336106870
H	-3.748089380	9.073719410	-1.547261440
C	-4.059448670	4.041814470	-1.857252880
H	-3.076553180	4.428231890	-2.143199120
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C	-5.033234120	9.970701370	-0.091022070
H	-4.596355620	10.960982560	-0.258950370
H	-6.098715090	10.111879720	0.122845680
H	-4.560162330	9.534960730	0.792726570
C	-4.687318890	3.417197370	-3.124431550
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H	-4.045791470	2.617111900	-3.512598010
H	-5.672091360	2.989565410	-2.902872260
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H	-3.156898690	2.201292720	-1.118529880
H	-3.370697950	3.446150190	0.133339180
H	-4.763763480	2.513612680	-0.445822640
S	-1.771814270	6.516671300	0.282501520
C	-1.914107320	8.193789790	0.936148670
C	-2.396036520	8.324898410	2.245732910
C	-1.505883500	9.325535500	0.220292610
C	-2.453731650	9.588980970	2.839570970
C	-1.586504820	10.586082070	0.815639940
C	-2.053556550	10.723421330	2.127018530
H	-2.731983230	7.446417490	2.791042570
H	-1.133122980	9.224903820	-0.794411080
H	-2.828948490	9.685530650	3.855512110
H	-1.277752660	11.463049640	0.251669560
H	-2.112269600	11.706587040	2.586323460
Au	-4.398383100	6.943164690	-4.904387900
Cl	-5.973295650	6.920187380	-6.595124370

4e

-16.57797630

C	-0.988993640	6.928020910	-2.413059230
C	-1.939138170	6.768567870	-1.441301890
N	-3.185522440	6.793386790	-2.109958490
C	-3.014994190	6.945340290	-3.455739960
N	-1.655120450	7.038615770	-3.624178340
H	0.086367270	6.971375550	-2.339730930
C	-1.021776100	7.276986530	-4.902066330
C	-0.640360370	6.169603670	-5.679434500
C	-0.851844010	8.611502020	-5.313456190
C	-0.034863340	6.436728740	-6.915169780
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C	0.167215720	7.747962260	-7.346185140
H	0.267411280	5.610156090	-7.552242290
H	-0.098070280	9.838525940	-6.916958720
H	0.633550320	7.933165280	-8.311003680
C	-1.365645030	9.785665240	-4.486312830
H	-1.723982000	9.396482880	-3.528250030
C	-0.925510210	4.736676850	-5.243421550
H	-1.311542480	4.763850910	-4.219592320
C	-0.254071190	10.810137110	-4.174667830
H	0.589388530	10.336084960	-3.659044140
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H	-0.645912160	11.609205000	-3.534175120
C	-2.575383190	10.447741040	-5.184870960
H	-2.986378920	11.247095600	-4.557207110
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H	-3.364740540	9.712287330	-5.371178650
C	0.351228250	3.869283010	-5.228728120
H	0.120271480	2.864803020	-4.855270280
H	0.774342760	3.761424690	-6.234018930
H	1.122041440	4.307676030	-4.584130720
C	-2.028877350	4.113481370	-6.129139190
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H	-2.937724360	4.723782500	-6.104644220
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C	-4.472829180	6.557462220	-1.491924380
C	-5.252656300	7.659473570	-1.097749220
C	-4.891155760	5.222182590	-1.349546090
C	-6.504823980	7.383334020	-0.531065810
C	-6.149697130	5.001474460	-0.775537310
C	-6.947684650	6.070798510	-0.369656390
H	-7.143859950	8.205256420	-0.222183690
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C	-4.805754530	9.098822070	-1.328358510
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C	-4.049520070	4.051907650	-1.846797390
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C	-5.512218190	9.691928970	-2.569923610
H	-5.147847270	10.707429880	-2.765697000
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H	-4.581312040	10.976831540	-0.253686480
H	-6.095539410	10.142032160	0.106443490
H	-4.575503320	9.553150380	0.803287070
C	-4.683038050	3.431648960	-3.113409660
H	-4.809851270	4.188335450	-3.894847990
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H	-5.668466650	3.006741630	-2.889684170
C	-3.815631840	2.996452960	-0.745367770
H	-3.149968320	2.207468840	-1.114682990
H	-3.357619870	3.449528690	0.140899110
H	-4.754287080	2.521940620	-0.437423240
S	-1.743178910	6.508829700	0.277486130
C	-1.918666520	8.177658480	0.937278070
C	-2.430761230	8.305152840	2.235452770

C	-1.509916190	9.317652640	0.234735970
C	-2.526076950	9.563798850	2.833304660
C	-1.622459270	10.579342600	0.818567960
C	-2.126693680	10.693228200	2.116364710
H	-2.767627910	7.425171890	2.777317790
H	-1.111240830	9.227312870	-0.770992860
H	-2.926655120	9.667969710	3.836831990
H	-1.318815380	11.467257740	0.272752900
Cl	-2.280640120	12.288928030	2.849323760
Au	-4.396149560	6.950788160	-4.895391820
Cl	-5.976249980	6.924906470	-6.580153680

4f

-17.02198393

C	-0.814358380	7.160193350	-2.606331980
C	-1.688897590	6.968662280	-1.572725510
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C	-2.899352710	6.965534910	-3.504633750
N	-1.564251980	7.154144750	-3.769604900
H	0.258344820	7.267940660	-2.598708630
C	-1.029374980	7.306503410	-5.107171330
C	-0.661827370	6.144613250	-5.809320370
C	-0.942400000	8.602465830	-5.645847350
C	-0.164313910	6.317163170	-7.108230020
C	-0.437998280	8.718207790	-6.948274610
C	-0.050265970	7.588939320	-7.669536090
H	0.123648340	5.446125220	-7.690080210
H	-0.361871500	9.700043640	-7.407076120
H	0.332428230	7.700009650	-8.681384480
C	-1.432557310	9.832353450	-4.889175730
H	-1.674017150	9.529193490	-3.865372670
C	-0.848720590	4.747946090	-5.226168170
H	-1.138302660	4.851171860	-4.175742040
C	-0.349959440	10.928552070	-4.795357820
H	0.565244060	10.544041230	-4.330587460
H	-0.087017880	11.318566970	-5.785153040
H	-0.715814110	11.768712460	-4.193616620
C	-2.735135360	10.370343160	-5.524965660
H	-3.118157470	11.219008340	-4.946234110
H	-2.557417660	10.708905440	-6.552200720
H	-3.504897580	9.592184690	-5.552918690
C	0.456796300	3.924937790	-5.258490080
H	0.300856550	2.953877430	-4.774717210
H	0.786813290	3.735937660	-6.286352760
H	1.266703280	4.444353190	-4.733553450
C	-2.003431160	4.014293920	-5.946986330
H	-2.179978130	3.037005470	-5.482880360
H	-2.929137270	4.596795380	-5.892926860
H	-1.764724250	3.853919740	-7.004797910
C	-4.220567100	6.754448250	-1.416368790
C	-4.918480470	7.949049450	-1.155440160
C	-4.680802250	5.482516970	-1.024613990
C	-6.100908280	7.845292710	-0.409842120
C	-5.865481190	5.439271390	-0.277179770
C	-6.560712600	6.608347750	0.037327980
H	-6.669807560	8.743139050	-0.185679990
H	-6.255971460	4.480260520	0.048499170
H	-7.479766300	6.550210370	0.616135460
C	-4.478037960	9.305061070	-1.700065940
H	-3.511162590	9.179099990	-2.196441410
C	-3.987612930	4.201620610	-1.475335700
H	-2.949062130	4.446991380	-1.714131300
C	-5.481718420	9.800723960	-2.767185510
H	-5.129380530	10.740160260	-3.207668770
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H	-3.973919540	11.311338810	-1.031646400
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C	-3.955325310	3.110498040	-0.388036380
H	-3.358121740	2.261330850	-0.738851900
H	-3.503665700	3.485872790	0.534082720
H	-4.959345830	2.731749760	-0.164007400
S	-1.190308130	6.619556810	0.107630880
C	-2.023062150	7.805959640	1.160220910
C	-3.276633490	7.490417450	1.694113040
C	-1.368297340	8.997487000	1.490829680
C	-3.893544860	8.389186670	2.562202550
C	-1.980872220	9.893900660	2.365701710
C	-3.240552790	9.581228450	2.888190870
H	-3.762557810	6.556369610	1.436869150
H	-0.385007340	9.206788910	1.081821240
H	-4.871379740	8.169875770	2.977562900
H	-1.492336690	10.823117250	2.640381680
O	0.240886300	6.916690260	0.123701510
O	-1.699621220	5.295532620	0.451708830
Cl	-4.026634940	10.721925000	3.970007000
Au	-4.383343560	6.900305150	-4.834716580
Cl	-6.089757470	6.834058230	-6.387446180

Crystallographic data

Crystal Structure Determination

9b and **9d** crystals were collected on a Bruker D8 diffractometer at room temperature, using Cu Kα radiation. Rawdata have been indexed and integrated using CrysAlis PRO.[22]

4a, **4b**, **4d**, **4e** and **5b** crystals data were collected at XRD2 beamline of the Elettra Synchrotron, Trieste (Italy),[23] using a monochromatic wavelength of 0.620 Å, at 100 K or 298 K. The data sets were integrated, scaled and corrected for Lorentz, absorption and polarization effects using XDS package.[24] The structures were solved by direct methods using SHELXT program[25] and refined using full−matrix least−squares implemented in SHELXL−2019/3.[26] Thermal motions for all non−hydrogen atoms have been treated anisotropically. Hydrogens have been included on calculated positions, riding on their carrier atoms. Geometric and thermal restrains (SAME, SADI, SIMU) have been applied to disordered fragments (e.g. solvent molecules). The Coot program was used for structure building.[27] The crystal data are given in Table 1SI. Pictures were prepared using Ortep3[28] and Pymol[29] software.

Crystallographic data have been deposited at the Cambridge Crystallographic Data Centre and allocated the deposition numbers CCDC 2518319 (**4a** at 100 K), 2518320 (**4a** at 298 K), 2518321 (**4b** at 100 K), 2518322 (**4b** at 298 K), 2518323 (**4d** at 100 K), 2518324 (**4d** at 298 K), 2518325 (**4e** at 100 K), 2518326 (**4e** at 298 K), 2518327 (**5b** at 100 K), 2518328 (**5b** at 298 K), 2518329 (**9b** at 273 K) and 2518330 (**9d** at 273 K). These data can be obtained free of charge via https://www.ccdc.cam.ac.uk/structures.

Table S1. Crystallographic data.

Compound	**4a@100 K**	**4a@298 K**	**4b@100 K**	**4b@298 K**	**4d@100 K**	**4d@298 K**
Formula	$AuC_{25}H_{34}ClN_2O_2 \cdot C_4H_{10}O$	$AuC_{25}H_{34}ClN_2O_2 \cdot C_4H_{10}O$	$AuC_{31}H_{46}ClN_2O_2$	$AuC_{31}H_{46}ClN_2O_2$	$AuC_{33}H_{40}ClN_2S \cdot C_4H_{10}O$	$AuC_{33}H_{40}ClN_2S \cdot C_4H_{10}O$
M/g·mol^{-1}	701.08	701.08	711.11	711.11	803.26	803.26
Space group	*P bca*	*P bca*	*P bca*	*P bca*	*P bca*	*P bca*
Crystal system	Orthorhombic	Orthorhombic	Orthorhombic	Orthorhombic	Orthorhombic	Orthorhombic
a/Å	15.363(3)	15.975(3)	17.342(3)	17.608(4)	18.885(4)	19.295(4)
b/Å	19.204(4)	19.624(4)	20.305(4)	20.463(4)	15.776(3)	16.015(3)
c/Å	20.595(4)	20.427(4)	36.449(7)	37.127(7)	24.371(5)	24.729(5)
α/°	90	90	90	90	90	90
β/°	90	90	90	90	90	90
γ/°	90	90	90	90	90	90
V/Å^3	6076(2)	6404(2)	12835(4)	13377(5)	7261(3)	7641(3)
Z	8	8	16	16	8	8
T/K	100(2)	298(2)	100(2)	298(2)	100(2)	298(2)
D_c/g·cm^{-3}	1.533	1.454	1.472	1.412	1.470	1.396
F(000)	2816	2816	5728	5728	3248	3248
μ/mm^{-1}	3.473	3.295	3.288	3.155	2.948	2.802
Measured Reflections	66247	83546	130125	228759	169771	179353
Unique Reflections	10321	13404	28114	29882	16171	16988
R_{int}	0.0470	0.0412	0.0829	0.0671	0.0940	0.0457
Obs. Refl.ns [I≥2σ(I)]	9306	6922	22830	17154	15007	14168
θ_{min}- θ_{max}/°	1.71 – 27.34	1.68 – 31.12	0.98 – 31.10	0.96 – 31.17	1.46 – 31.15	1.44 – 31.16
hkl ranges	-22,22; -28,27; -29,30	-21,22; -30,29; -31,29	-27,24; -31,24; -52,52	-28,28; -29,31; -54,55	-29,29; -24,24; -34,35	-29,28; -26,26; -37,37
R(F^2) (Obs.Refl.ns)	0.0259	0.0408	0.0410	0.0526	0.0289	0.0277
wR(F^2) (All Refl.ns)	0.0735	0.1446	0.1100	0.1749	0.0756	0.0806
No. Variables	336	329	688	688	399	399
Goodness of fit	1.049	0.996	1.027	1.025	1.039	1.035
$\Delta\rho_{max}$; $\Delta\rho_{min}$/e·Å^{-3}	2.56; -1.29	2.17; -1.22	2.37; -2.05	1.80; -0.93	1.72; -2.02	0.97; -1.17
CCDC Deposition N.	2518319	2518320	2518321	2518322	2518323	2518324

Compound	**4e@100 K**	**4e@298 K**	**5b@100 K**	**5b@298 K**	**9b@273 K**	**9d@273 K**
Formula	$AuC_{33}H_{39}Cl_2N_2S \cdot CHCl_3$	$AuC_{33}H_{39}Cl_2N_2S \cdot CHCl_3$	$AuC_{32}H_{41}N_2O_3$	$AuC_{32}H_{41}N_2O_3$	$AuC_{37}H_{50}ClN_2O_2S$	$AuC_{39}H_{44}ClN_2S_2$
M/g·mol^{-1}	882.95	882.95	698.63	698.63	819.26	837.30
Space group	*P bca*	*P bca*	*P nma*	*P nma*	*P* $2_1/c$	*P* -1
Crystal system	Orthorhombic	Orthorhombic	Orthorhombic	Orthorhombic	Monoclinic	Triclinic
a/Å	17.559(4)	17.755(4)	17.435(3)	17.569(4)	15.6679(6)	9.7668(2)
b/Å	17.582(4)	17.963(4)	8.602(2)	8.782(2	12.8012(4)	10.9121(2)
c/Å	23.746(5)	24.030(5)	19.950(4)	20.365(4)	19.3550(6)	18.4252(4)
α/°	90	90	90	90	90	88.475(1)
β/°	90	90	90	90	95.731(1)	77.522(1)
γ/°	90	90	90	90	90	76.577(1)
V/Å^3	7331(3)	7664(3)	2992.0(10)	3142.1(11)	3862.6(2)	1864.36(7)
Z	8	8	4	4	4	2
T/K	100(2)	298(2)	100(2)	298(2)	100(2)	100(2)
D_c/g·cm^{-3}	1.600	1.530	1.551	1.477	1.409	1.492
F(000)	3504	3504	1400	1400	1656	840
μ/mm^{-1}	3.111	2.975	3.470	3.304	8.536	9.329
Measured Reflections	165721	70594	19295	58644	85711	35582
Unique Reflections	17116	16667	5685	7623	7614	7200
R_{int}	0.1097	0.0779	0.0519	0.0623	0.0406	0.0412
Obs. Refl.ns [I≥2σ(I)]	14859	8022	5073	3921	7135	7182
θ_{min}- θ_{max}/°	1.50 – 31.11	1.48 – 31.15	1.35 – 28.01	1.33 – 31.12	4.15 – 72.36	4.15 – 72.36
hkl ranges	-27,26; -27,24; -39,38	-29,29; -28,29; -36,35	-26,25; -8,13; -30,3	-29,29; -14,14; -32,32	-19,19; -15,15; -23,23	-11,12; -13,13; -22,22
R(F^2) (Obs.Refl.ns)	0.0320	0.0570	0.0483	0.0537	0.0306	0.0392
wR(F^2) (All Refl.ns)	0.0795	0.2078	0.1225	0.1962	0.0725	0.0985
No. Variables	397	397	304	305	407	415
Goodness of fit	1.067	0.999	1.134	1.028	1.105	1.176
$\Delta\rho_{max}$; $\Delta\rho_{min}$/e·Å^{-3}	1.66; -2.72	2.20; -3.00	1.58; -2.02	1.28; -0.60	0.67; -1.33	1.84; -2.39
CCDC Deposition N.	2518325	2518326	2518327	2518328	2518329	2518330

Table S2. Selected metal distances and angles for **4a** at 100 K and 298 K. Corresponding naming scheme in use is reported (hydrogens omitted for clarity).

4a – $AuC_{25}H_{34}ClN_2O_2$							
100 K				**298 K**			
Distances	**(Å)**	**Angles**	**(°)**	**Distances**	**(Å)**	**Angles**	**(°)**
Au_1-Cl_2	2.272(1)	C1_3-Au_1-Cl_2	177.33(6)	Au_1-Cl_2	2.265(1)	C1_3-Au_1-Cl_2	178.5(1)
Au_1-C1_3	1.969(2)			Au_1-C1_3	1.981(3)		

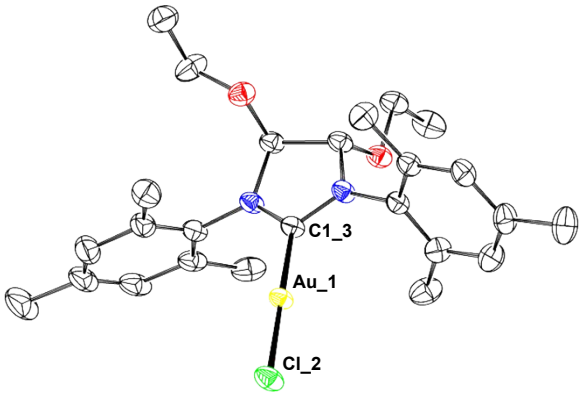


Table S3. Selected metal distances and angles for **4b** at 100 K and 298 K. Corresponding naming scheme in use is reported (hydrogens omitted for clarity).

4b – $AuC_{31}H_{46}ClN_2O_2$							
100 K				**298 K**			
ASU MOLECULE 1				**ASU MOLECULE 1**			
Distances	**(Å)**	**Angles**	**(°)**	**Distances**	**(Å)**	**Angles**	**(°)**
Au_1-Cl_2	2.278(1)	C1_3-Au_1-Cl_2	176.65(7)	Au_1-Cl_2	2.269(2)	C1_3-Au_1-Cl_2	177.4(1)
Au_1-C1_3	1.972(2)			Au_1-C1_3	1.967(4)		
ASU MOLECULE 2				**ASU MOLECULE 2**			
Distances	**(Å)**	**Angles**	**(°)**	**Distances**	**(Å)**	**Angles**	**(°)**
Au_1-Cl_2	2.266(1)	C1_3-Au_1-Cl_2	178.03(7)	Au_1-Cl_2	2.263(2)	C1_3-Au_1-Cl_2	179.0(1)
Au_1-C1_3	1.967(2)			Au_1-C1_3	1.962(3)		

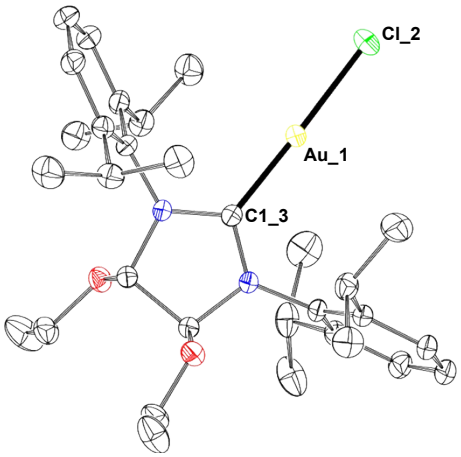

Cl_2
Au_1
C1_3

Table S4. Selected metal distances and angles for **4d** at 100 K and 298 K. Corresponding naming scheme in use is reported (hydrogens omitted for clarity).

4d – $AuC_{33}H_{40}ClN_2S$							
100 K				**298 K**			
Distances (Å)		**Angles (°)**		**Distances (Å)**		**Angles (°)**	
Au_1-Cl_2	2.270(1)	C1_3-Au_1-Cl_2	178.14(4)	Au_1-Cl_2	2.263(1)	C1_3-Au_1-Cl_2	178.93(5)
Au_1-C1_3	1.968(1)			Au_1-C1_3	1.968(2)		

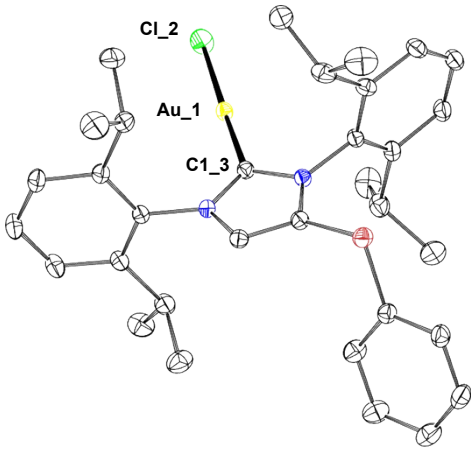


Table S5. Selected metal distances and angles for **4e** at 100 K and 298 K. Corresponding naming scheme in use is reported (hydrogens omitted for clarity).

4e – $AuC_{33}H_{39}Cl_2N_2S$							
100 K				**298 K**			
Distances (Å)		**Angles (°)**		**Distances (Å)**		**Angles (°)**	
Au_1-Cl_2	2.273(1)	C1_3-Au_1-Cl_2	175.86(5)	Au_1-Cl_2	2.268(1)	C1_3-Au_1-Cl_2	177.9(1)
Au_1-C1_3	1.971(2)			Au_1-C1_3	1.971(4)		

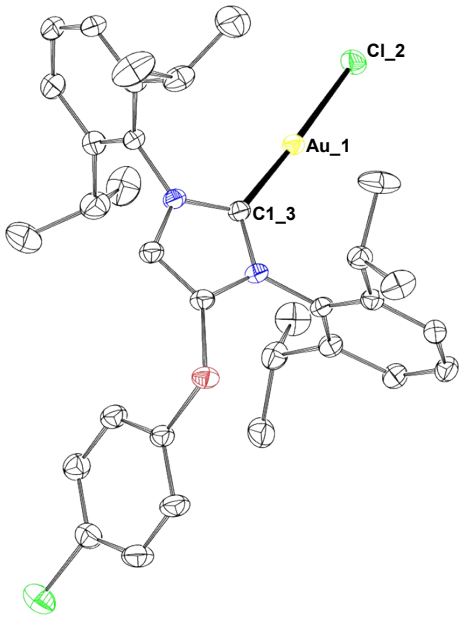


Table S6. Selected metal distances and angles for **5b** at 100 K and 298 K. Corresponding naming scheme in use is reported (hydrogens omitted for clarity).

5b – $AuC_{25}H_{34}ClN_2O_2$							
100 K				**298 K**			
Distances	**(Å)**	**Angles**	**(°)**	**Distances**	**(Å)**	**Angles**	**(°)**
Au_1-C4_2	2.085(4)	C1_3-Au_1-C4_2	176.3(2)	Au_1-C4_2	2.074(4)	C1_3-Au_1-C4_2	176.7(2)
Au_1-C1_3	2.055(6)	NHC-Ph Ave Plane[a]	41.7(3)	Au_1-C1_3	2.056(6)	NHC-Ph Ave Plane[a]	45.6(3)

[a]Average angle between the mean NHC plane and phenyl ligand core.

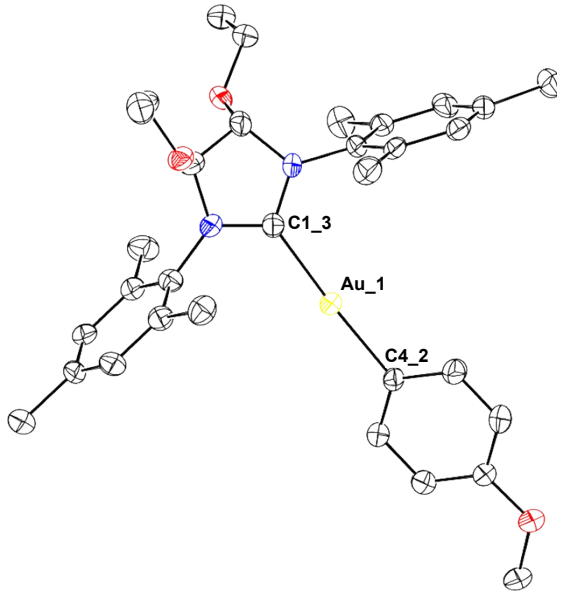


Table S7. Selected metal distances and angles for **9b** at 273 K. Corresponding naming scheme in use is reported (hydrogens omitted for clarity).

9b (273 K) – $AuC_{37}H_{50}ClN_2O_2S$

Distances	(Å)	**Angles**	(°)
Au_1-S_2	2.291(1)	C1_3-Au_1-S_2	179.14(9)
Au_1-C1_3	2.023(3)	NHC-Ph Ave Plane[a]	19.0(1)

[a]Average angle between the mean NHC plane and phenyl ligand core.

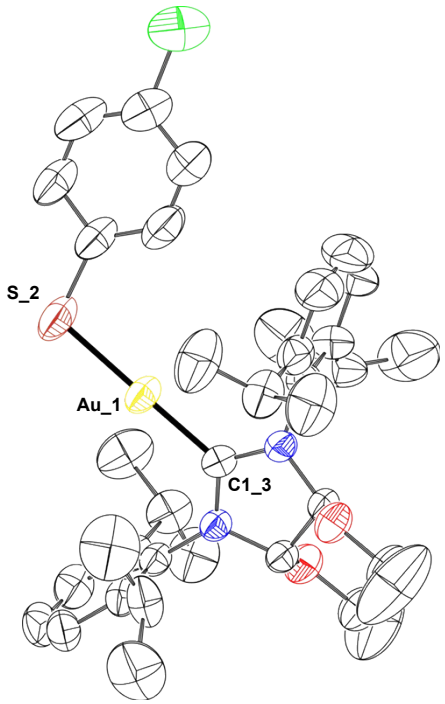
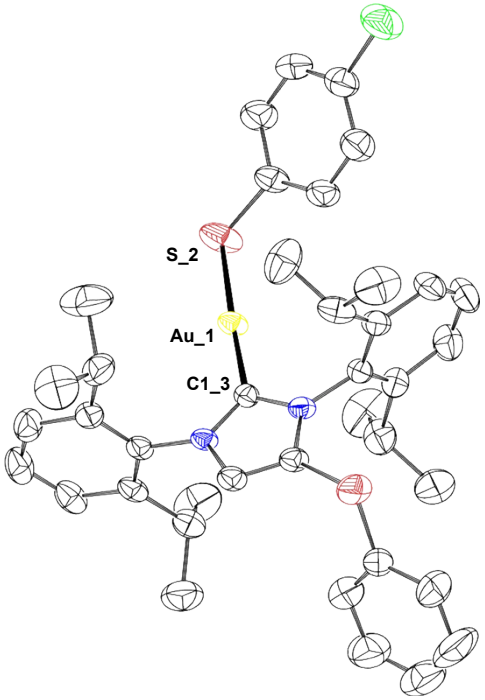


Table S8. Selected metal distances and angles for **9d** at 273 K. Corresponding naming scheme in use is reported (hydrogens omitted for clarity).

9d (273 K) – $AuC_{39}H_{44}ClN_2S_2$

Distances	(Å)	**Angles**	(°)
Au_1-S_2	2.293(1)	C1_3-Au_1-S_2	176.5(1)
Au_1-C1_3	2.013(4)	NHC-Ph Ave Plane[a]	43.3(2)

[a]Average angle between the mean NHC plane and phenyl ligand core.

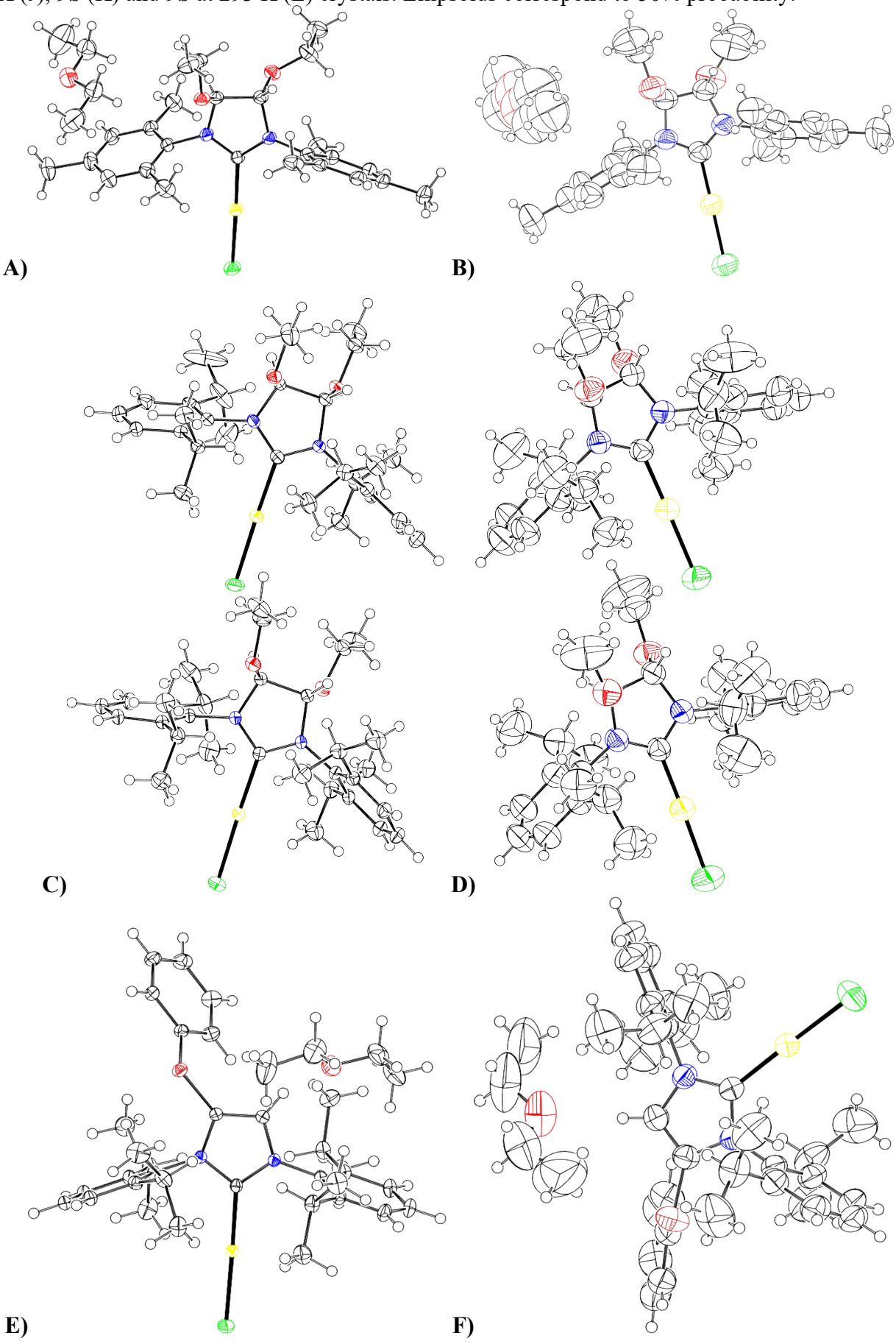


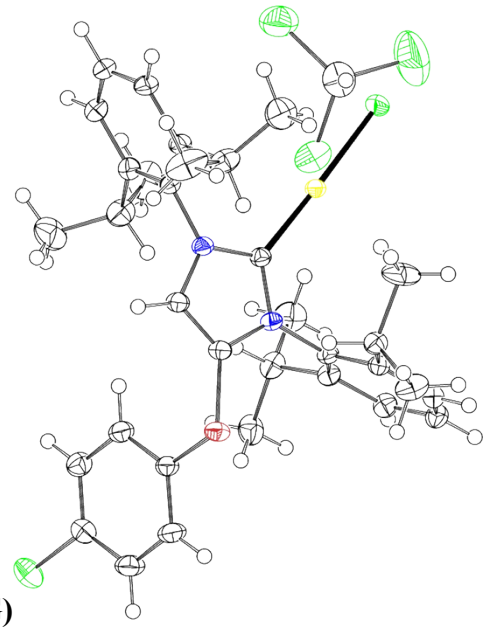
Structural characterization.

4a, **4b**, **4d**, **4e**, **5b**, **9b** and **9d** molecules have been crystallized, characterized through XRD and show typical linear Au(I) coordination (Tables S2-S8). All crystal forms bear one crystallographically independent molecule, except for **4b**, where two almost superimposable moieties have been found (Figure S2B; R.M.S.D. < 0.4 Å). Significant Au-ligand bond elongation is detected going from phenyl (d_{Au-C} = 2.06(1) Å) to S-phenyl (d_{Au-S} = 2.29(1) Å) and Cl (d_{Au-Cl} = 2.27(1) Å), with corresponding loosening of Au-NHC bonds (spanning from d_{Au-NHC} = 1.97(1) Å to d_{Au-NHC} = 2.06(1) Å). These changes are mostly due to differences in ligands electron donor properties, since steric hindrances of NHC N-substituents are similar, among different molecules. Negligible effects on gold coordination environments can be measured changing NHC carbon backbone substituents or considering different molecular packing (Figure S3).

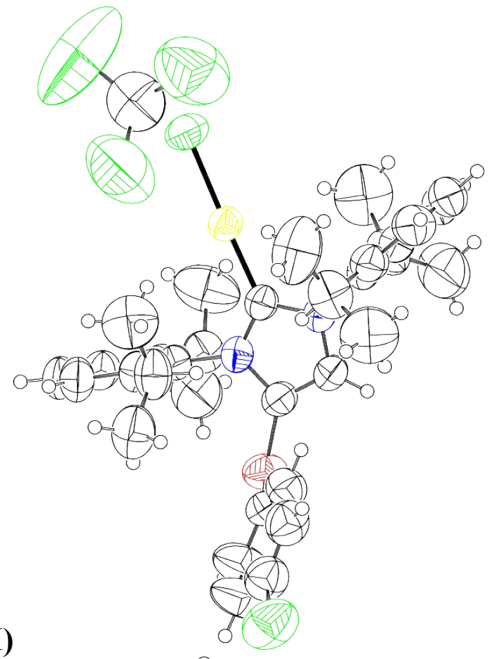
Crystal packing show hydrophobic contacts among neighbour molecules, through weak intermolecular CH···π and π···π interactions, involving NHC substituents. Solvent molecules (chloroform or diethyl ether) have been found in crystal packing of **4a**, **4d** and **4e** (Figure S1A-B, E-H), filling hydrophobic pockets. Formation of an intramolecular CH···π interaction has been found in **9b** and **9d**, between benzenethiol and neighbour Dipp NHC substituents, locking the sulphur containing ligand in superimposable orientations for both complexes ($d_{CH\cdots\pi}$ = 3.777(4) Å, $\Lambda_{CH\cdots\pi}$ = 149°; Figure S3B). Minor cell volume contraction has been found upon cooling (< 7%), with no significant packing and molecular rearrangements, as shown through models overlap in Figure S2 (R.M.S.D. < 0.5 Å).

Figure S1. Ortep representations of molecular models for **4a** at 100 K (A) and 298 K (B), **4b** at 100 K (C) and 298 K (D), **4d** at 100 K (E) and 298 K (F), **4e** at 100 K (G) and 298 K (H), **5b** at 100 K (I) and 298 K (J), **9b** (K) and **9b** at 293 K (L) crystals. Ellipsoids correspond to 50% probability.

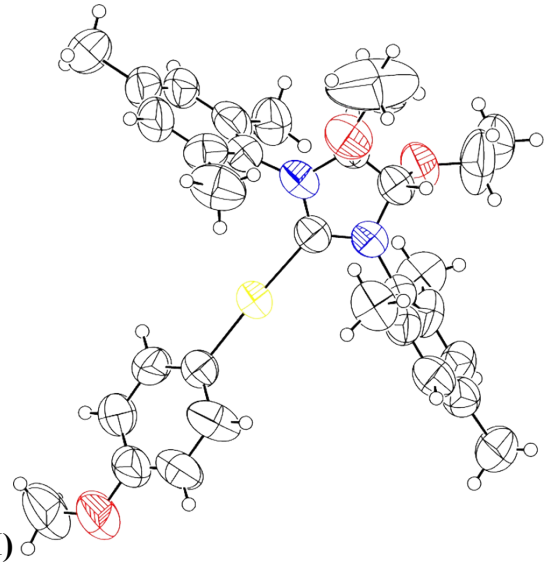




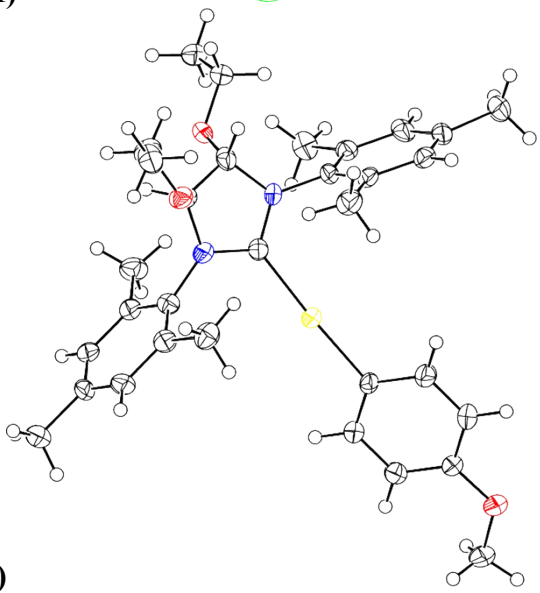
G)



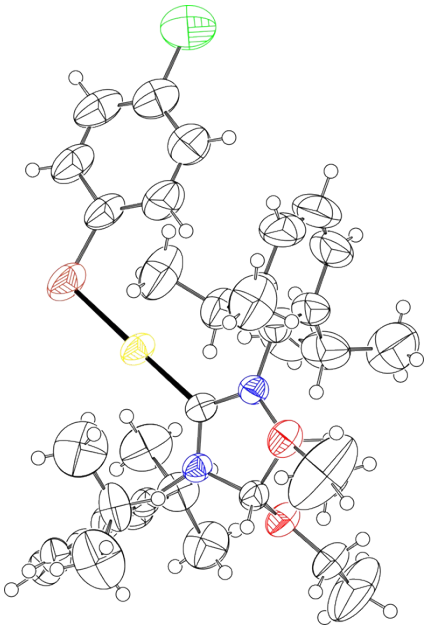
H)



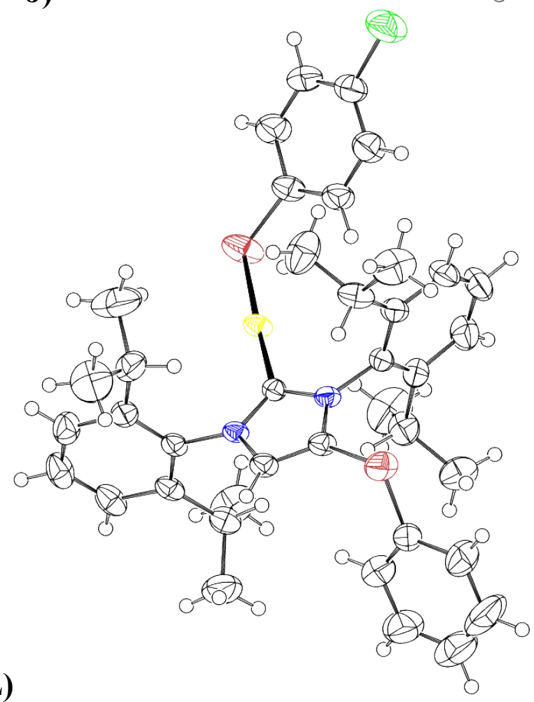
I)



J)



K)



L)

Figure S2. Superimposition of **4a** (A), **4b** (B), **4d** (C), **4e** (D) and **5b** (E) crystallographically independent molecules, obtained at different temperatures (yellow sticks for data collected at 100 K and magenta sticks for 298 K). Hydrogens omitted for clarity.

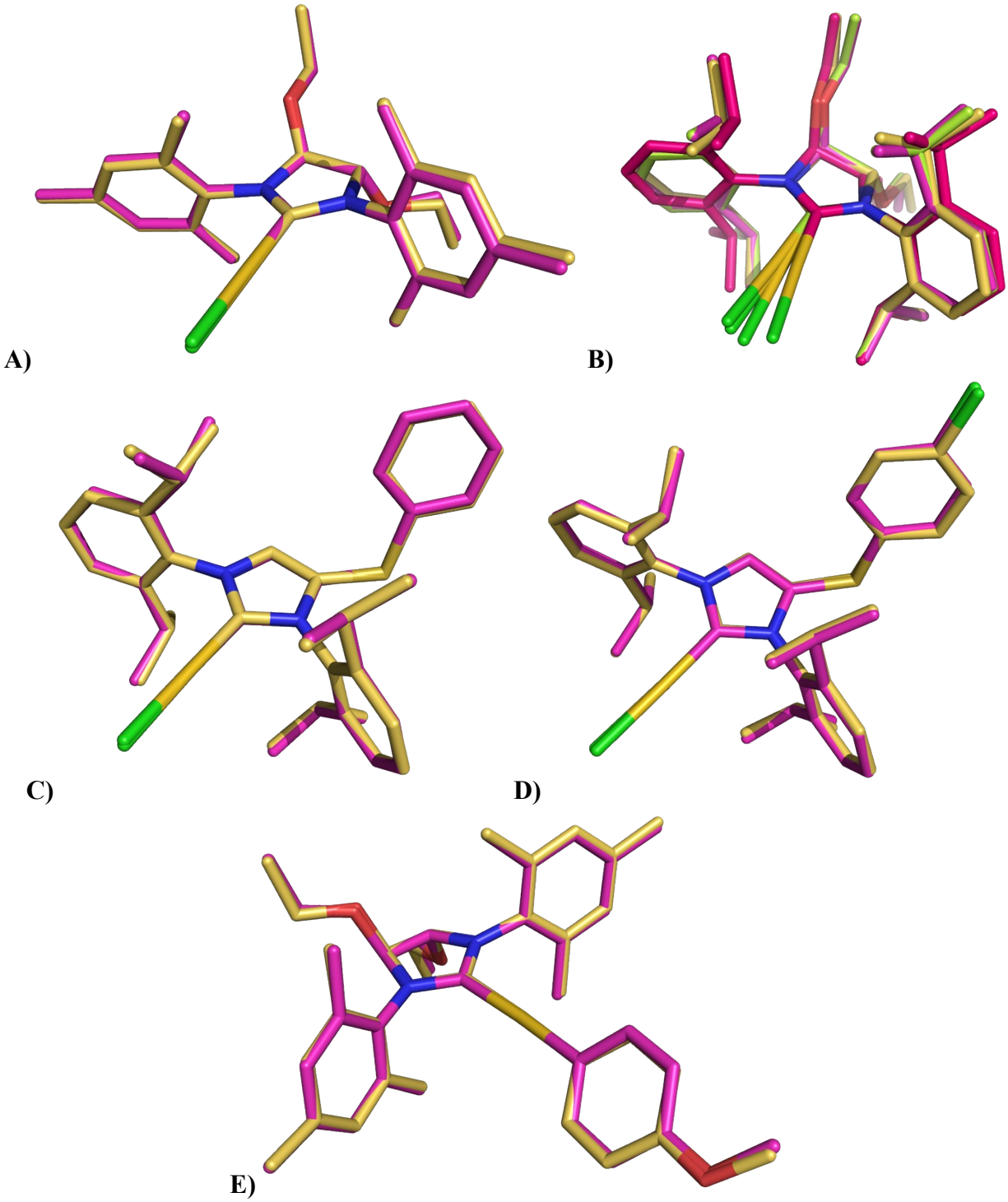
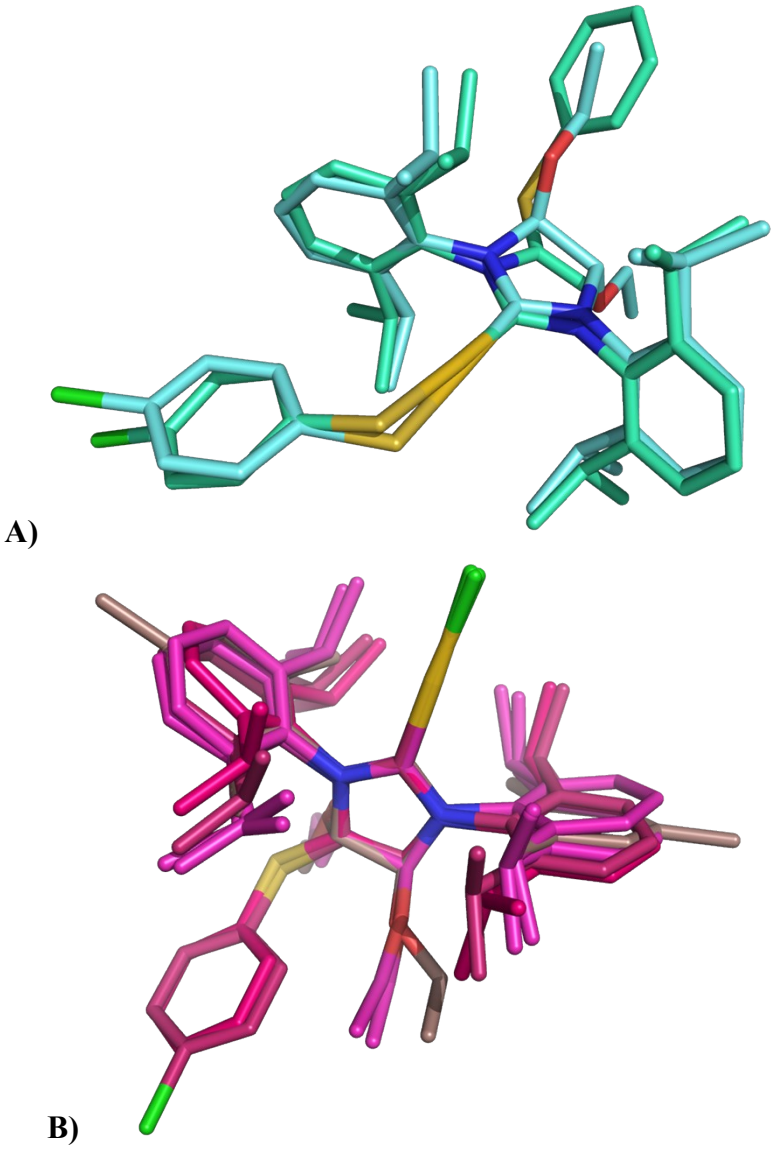


Figure S3. Superimposition of: A) **9b** and **9d** (shades of cyan sticks) and B) **4a**, **4b**, **4d**, **4e** models (shades of pink sticks), determined at 100 K. R.M.S.D. among common atoms is < 1.5 Å. Hydrogens omitted for clarity.



A)

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References

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