Supporting Information

Gold(I) phosphine derivatives with improved selectivity as topically active drug leads to overcome 5-nitroheterocyclic drug resistance in *Trichomonas vaginalis*

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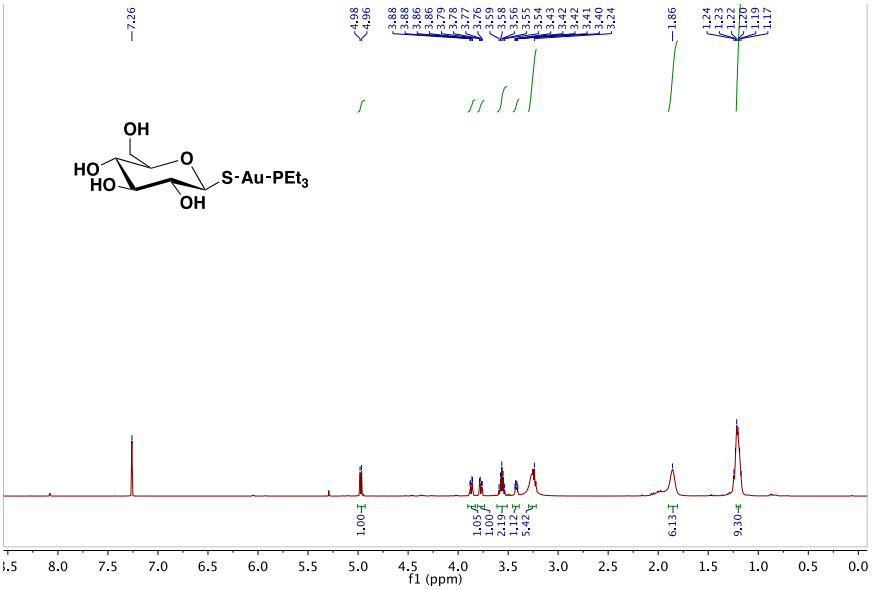
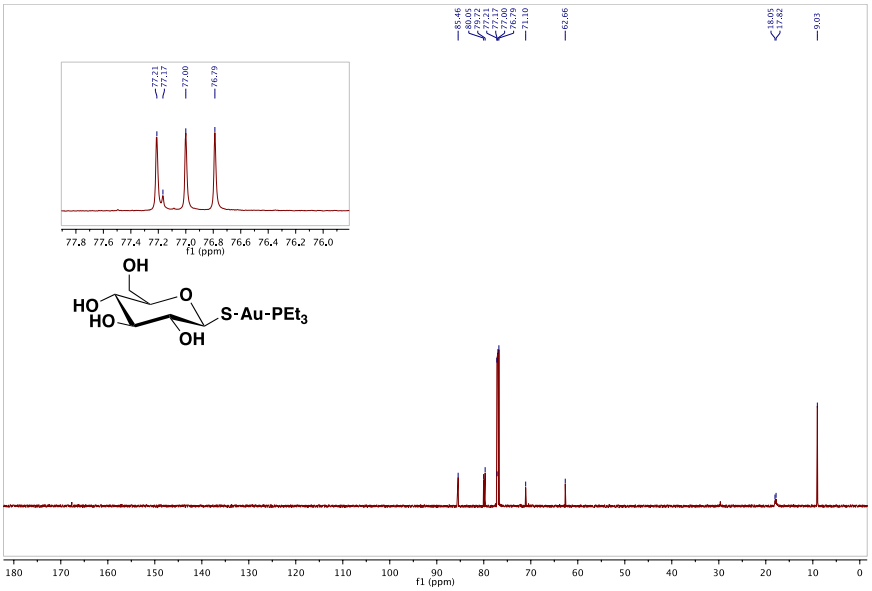
(1-Thio-*β*-D-glucopyranosato)(triethylphosphine) gold(I) (1)

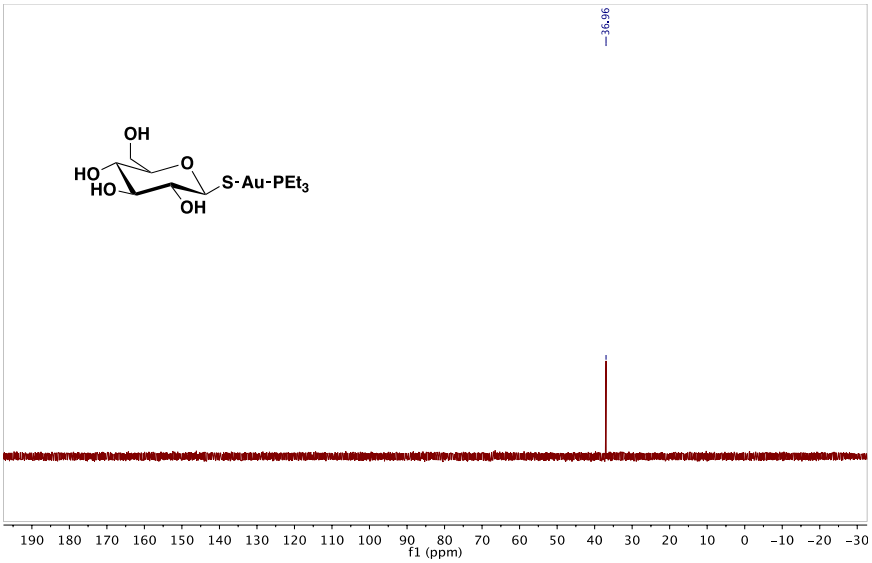
^{1}H NMR ($CDCl_3$, 600 MHz)



^{13}C{^{1}H} NMR ($CDCl_3$, 151 MHz)

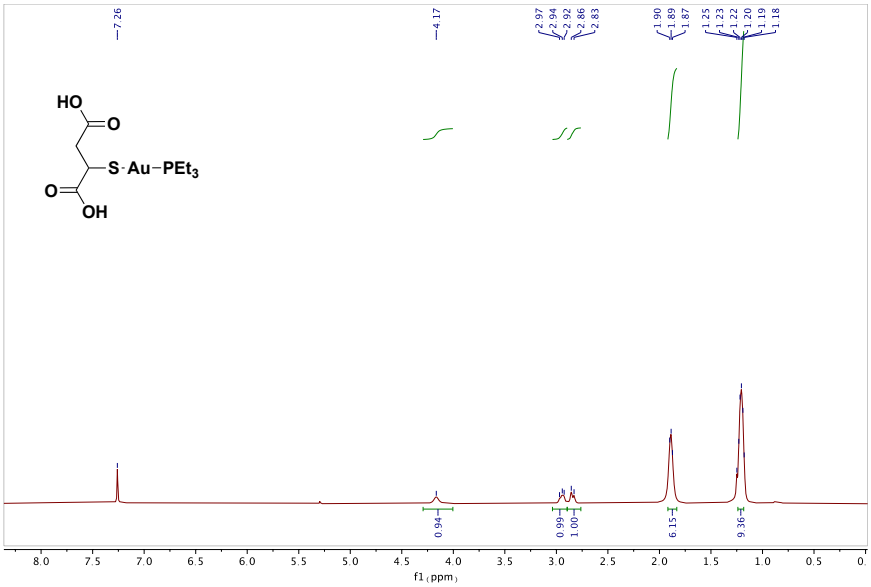


^{31}P{^{1}H} NMR ($CDCl_3$, 243 MHz)

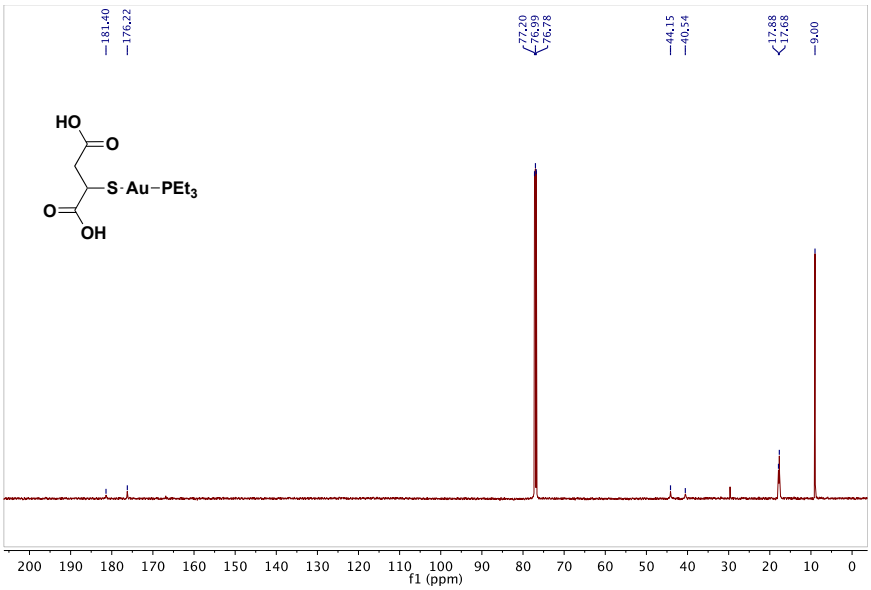


S-Triethylphosphine gold(I) thiomalic acid (2)

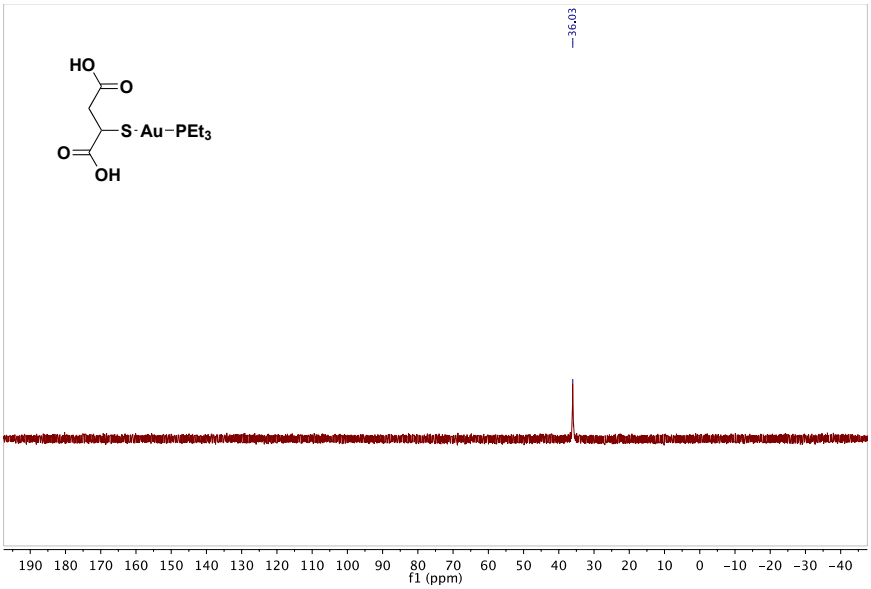
^{1}H NMR ($CDCl_3$, 600 MHz)



$^{13}C\{^{1}H\}$ NMR ($CDCl_3$, 151 MHz)

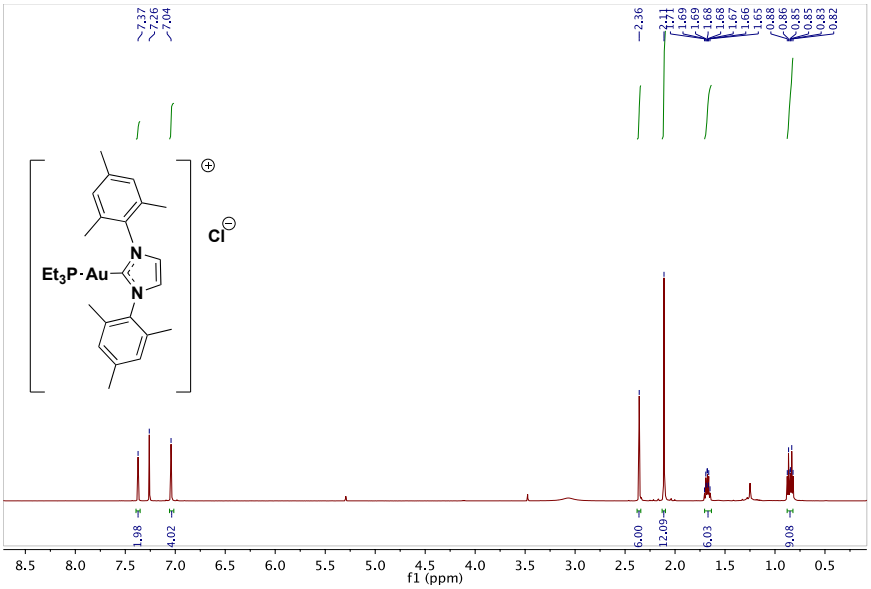


$^{31}P\{^{1}H\}$ NMR ($CDCl_3$, 243 MHz)

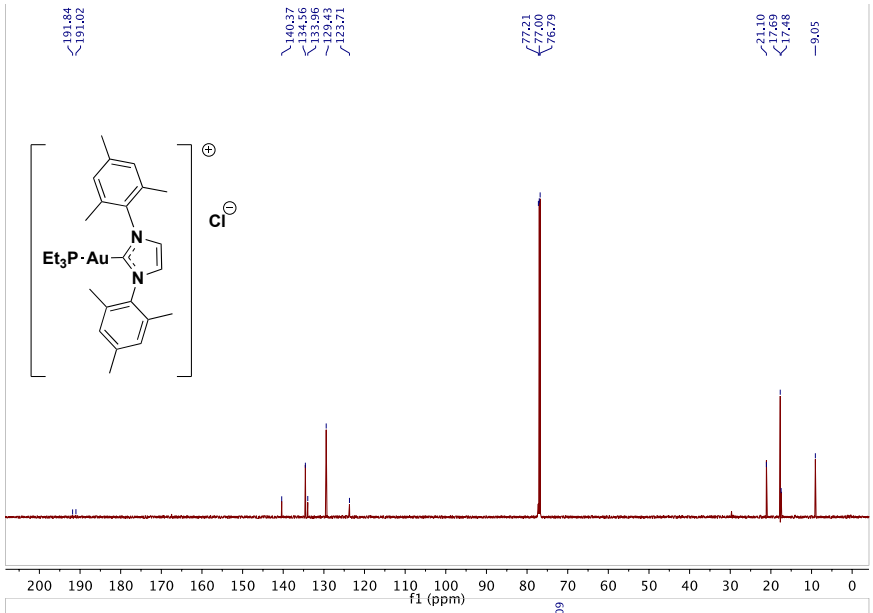


[Triethylphosphine-(bis(2,4,6-trimethylphenyl)imidazol-2-ylidene)]gold(I) chloride (3)

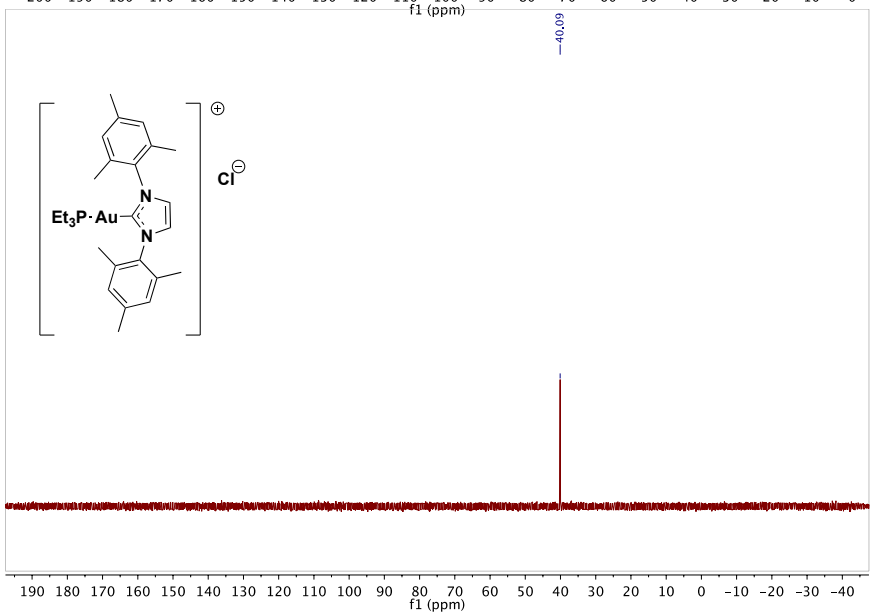
^{1}H NMR ($CDCl_3$, 600 MHz)



^{13}C{^{1}H} NMR ($CDCl_3$, 151 MHz)

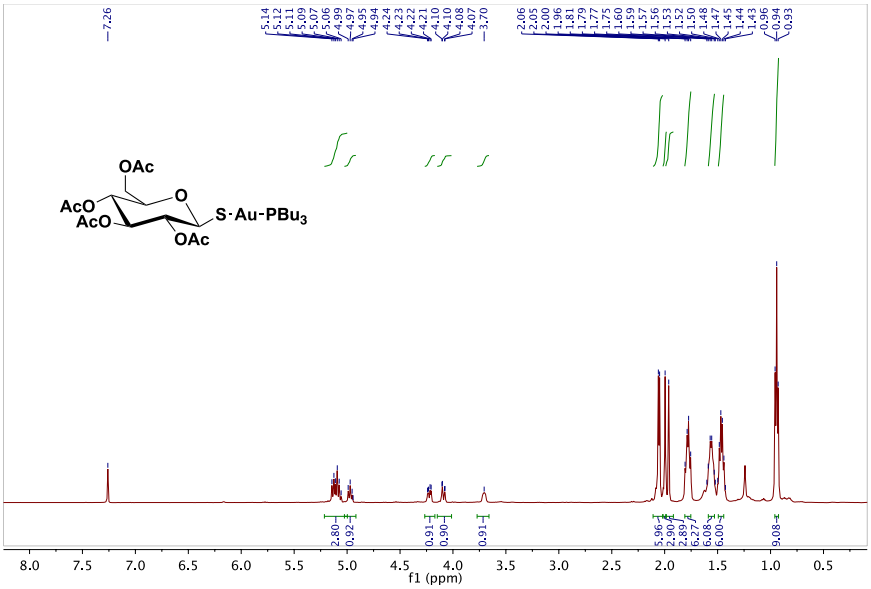


^{31}P{^{1}H} NMR ($CDCl_3$, 243 MHz)

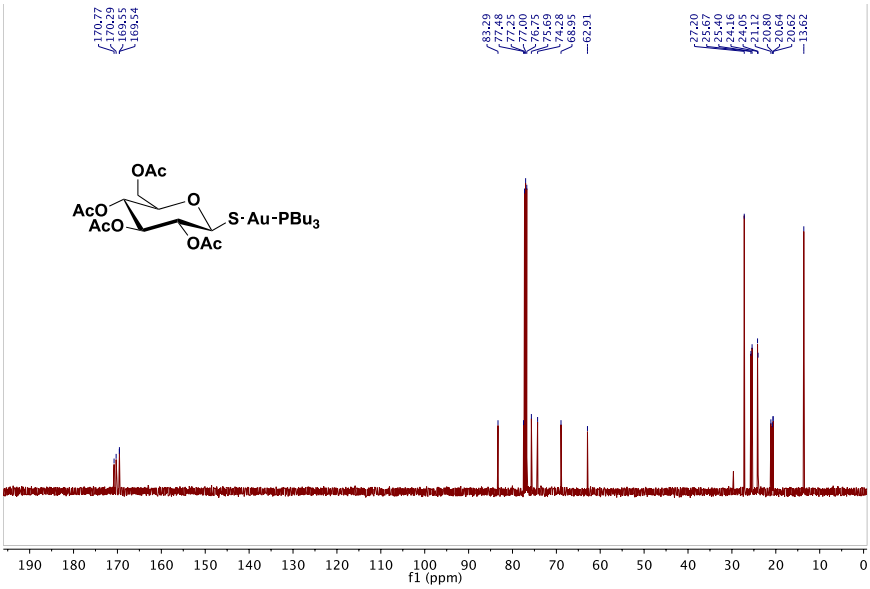


2,3,4,6-Tetra-O-acetyl-1-thio-*β*-D-galacotopyranosato)(butylphosphine) gold(I) (5)

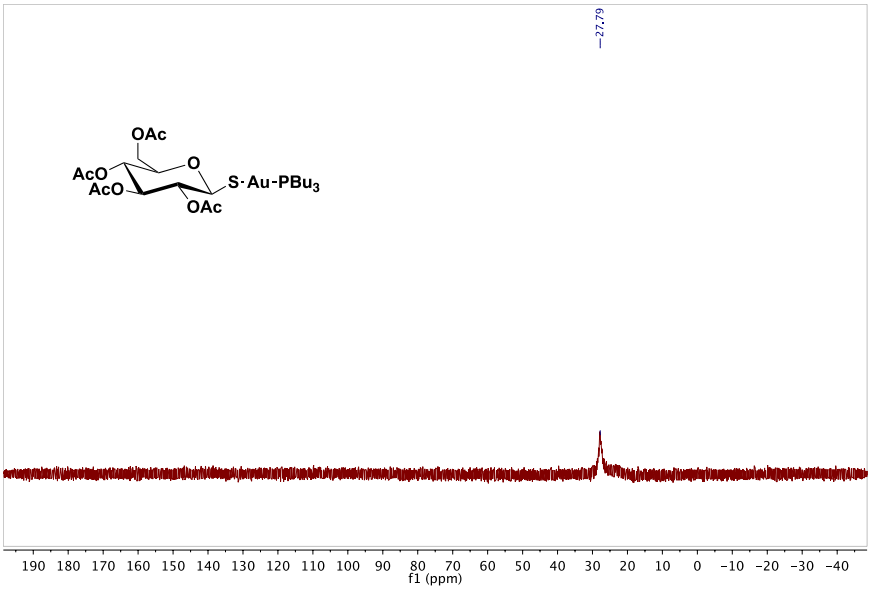
^{1}H NMR ($CDCl_3$, 500 MHz)



^{13}C{^{1}H} NMR ($CDCl_3$, 126 MHz)



^{31}P{^{1}H} NMR ($CDCl_3$, 202 MHz)



(1-Thio-*β*-D-glucopyranosato)(tributylphosphine) gold(I) (6)

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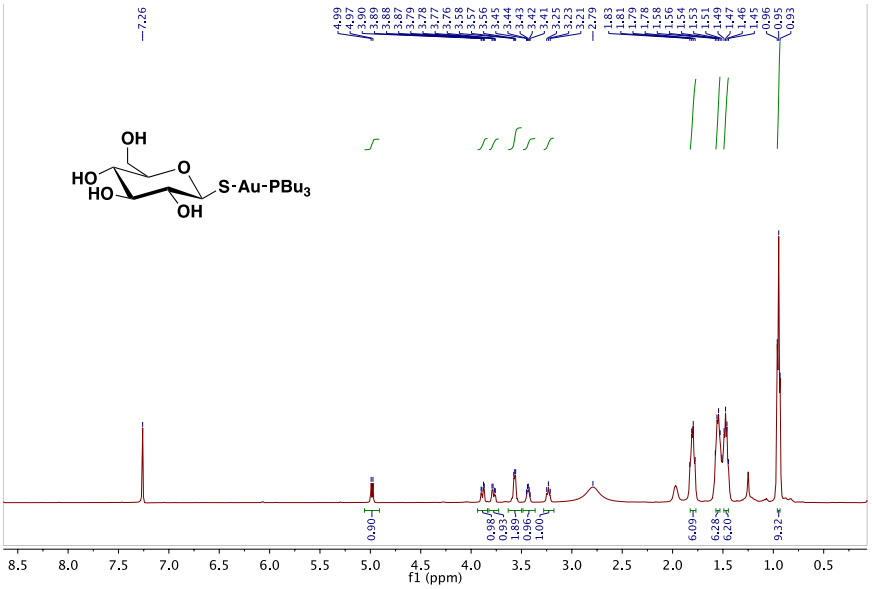
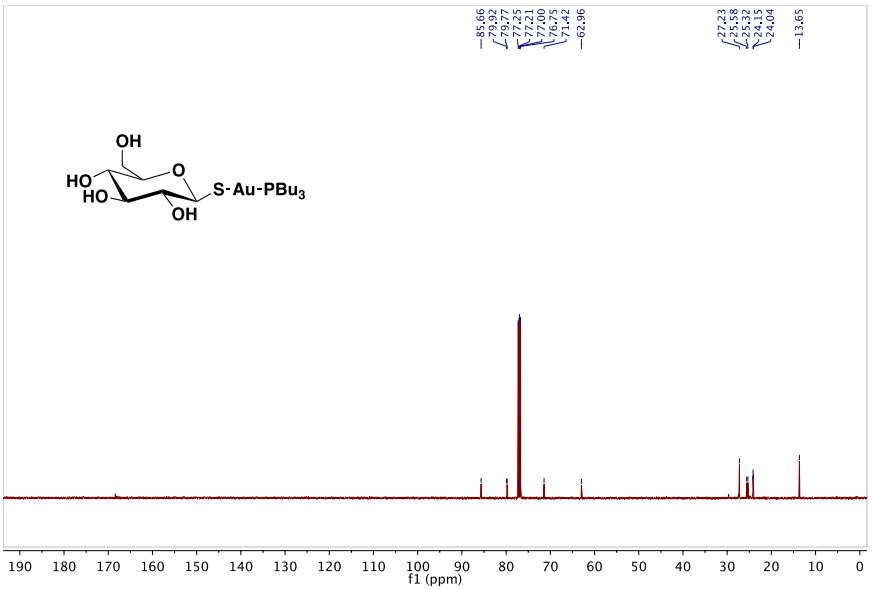
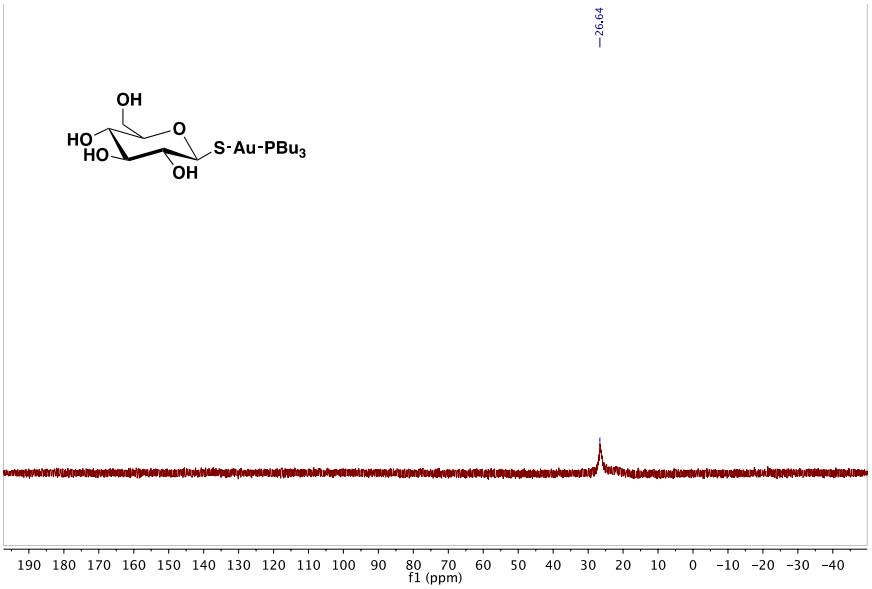


^{13}C{^{1}H} NMR ($CDCl_3$, 126 MHz)

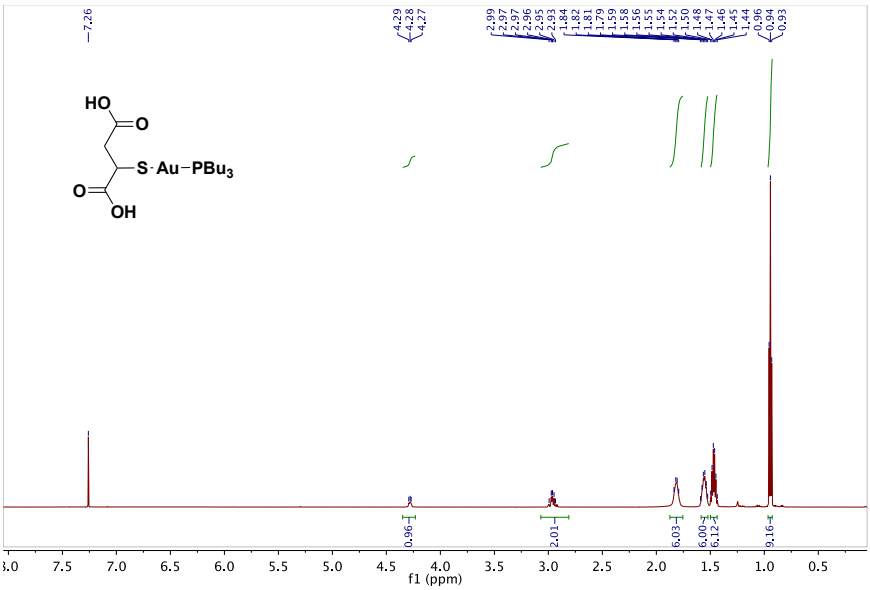


^{31}P{^{1}H} NMR ($CDCl_3$, 202 MHz)

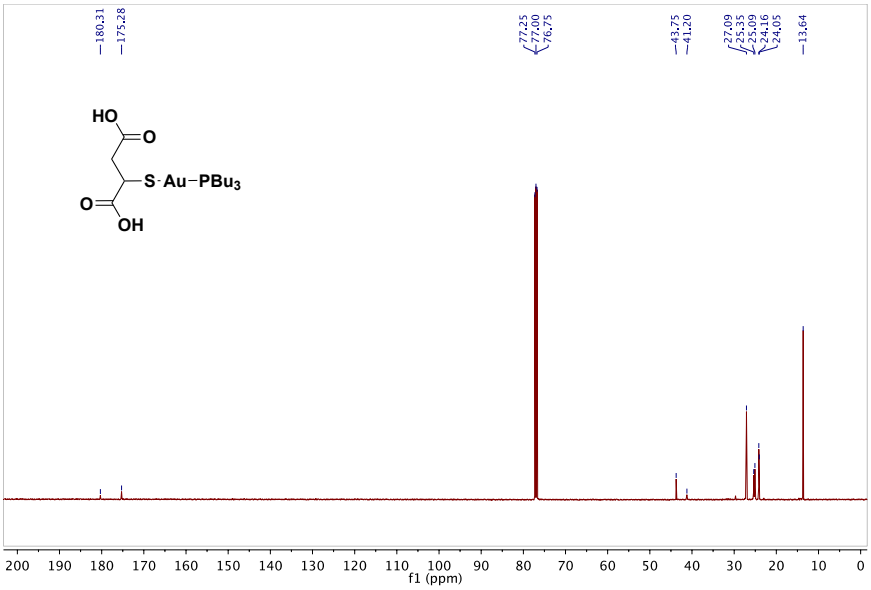


S-Tributylphosphine gold(I) thiomalic acid (7)

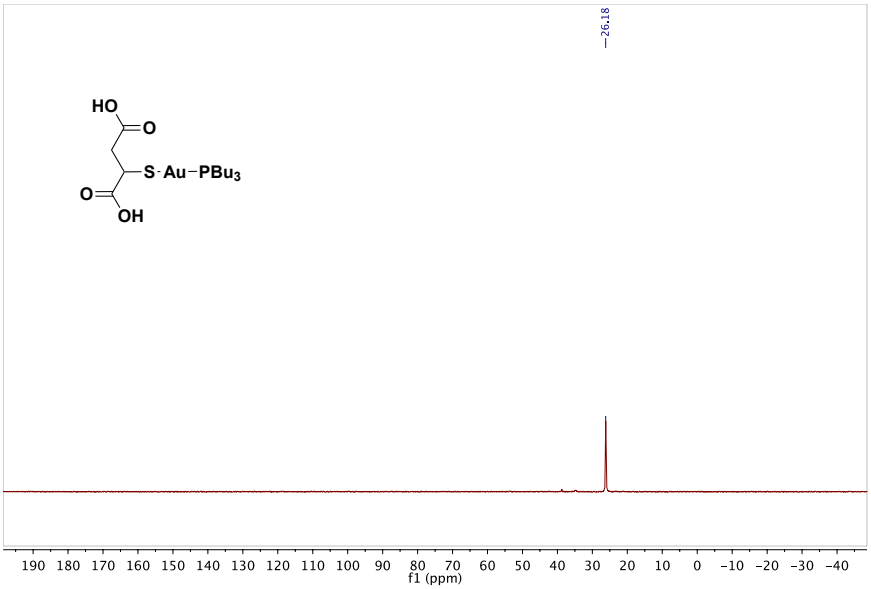
^{1}H NMR ($CDCl_3$, 600 MHz)



^{13}C{^{1}H} NMR ($CDCl_3$, 126 MHz)

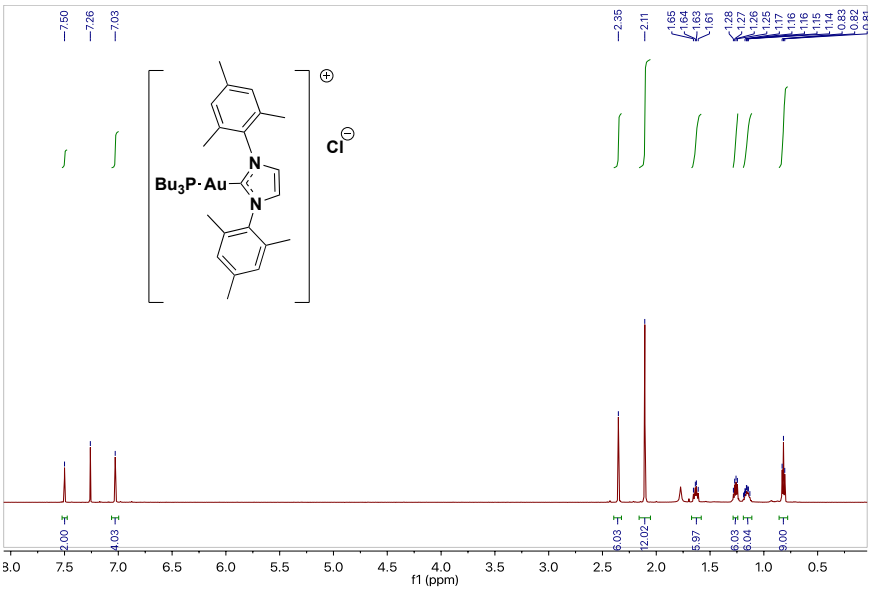


^{31}P{^{1}H} NMR ($CDCl_3$, 202 MHz)

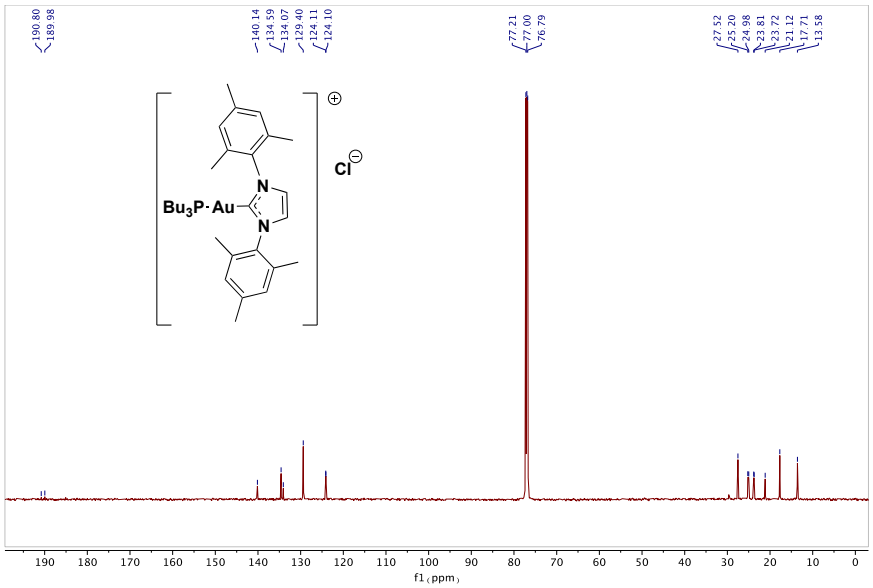


[Tributylphosphine-(bis(2,4,6-trimethylphenyl)imidazol-2-ylidene)]gold(I) chloride (8)

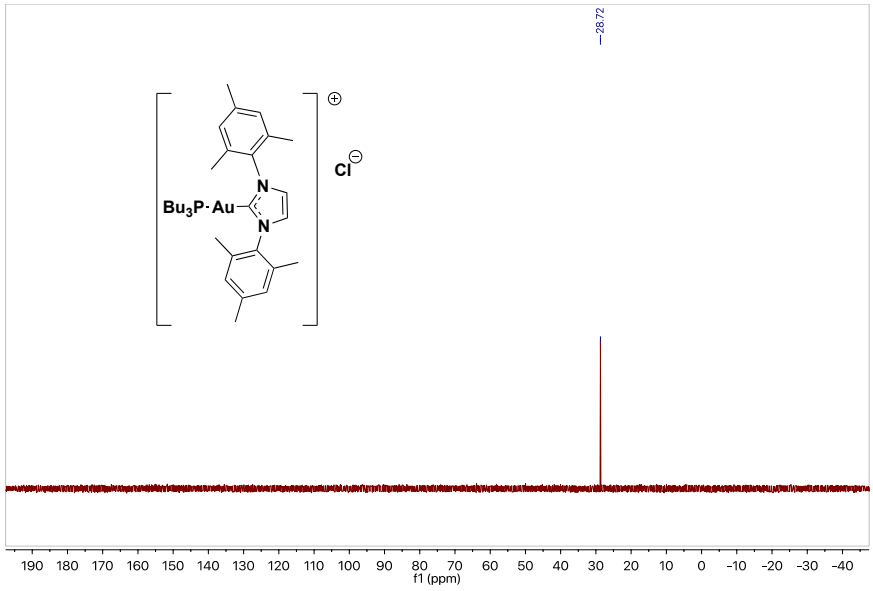
^{1}H NMR ($CDCl_3$, 600 MHz)



^{13}C{^{1}H} NMR ($CDCl_3$, 151 MHz)

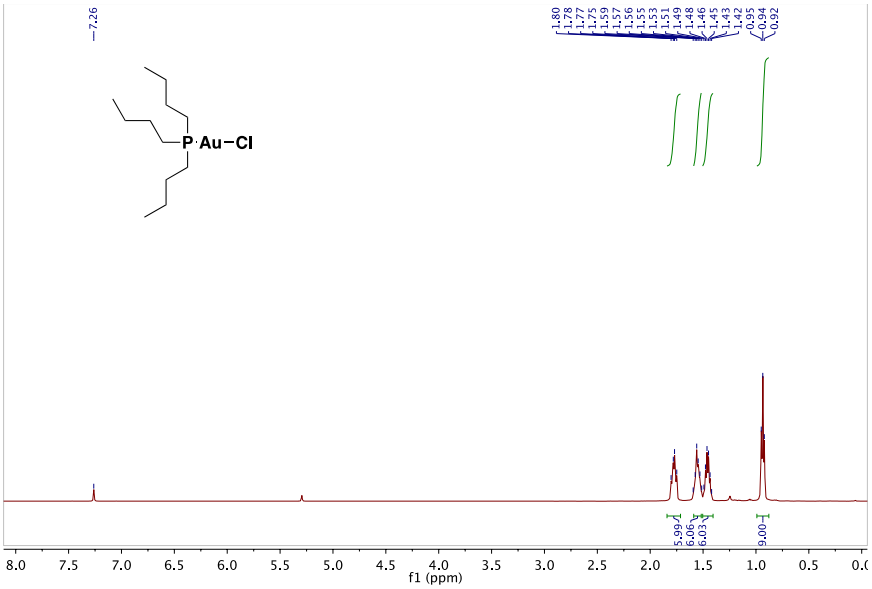


^{31}P{^{1}H} NMR ($CDCl_3$, 243 MHz)

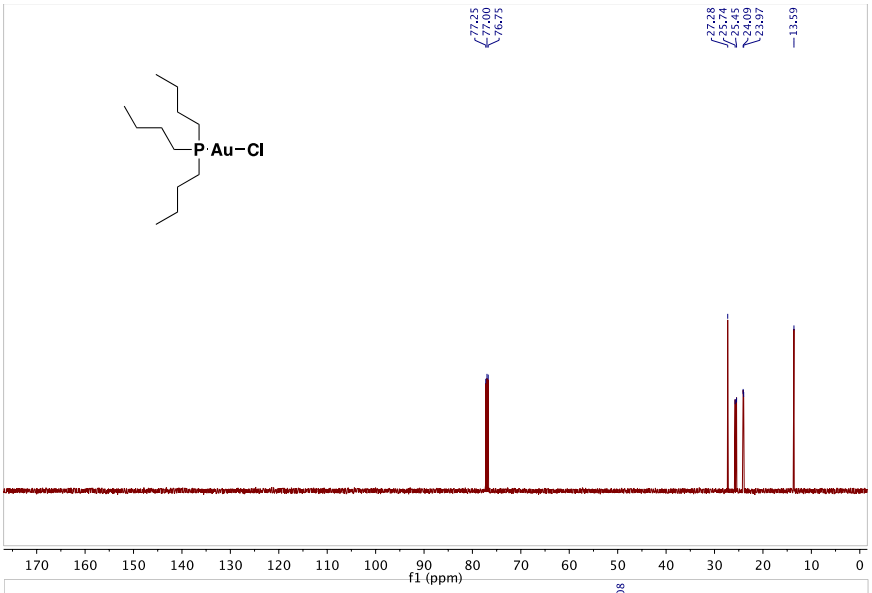


(Tri-*n*-butylphosphine)gold(I) chloride (9)

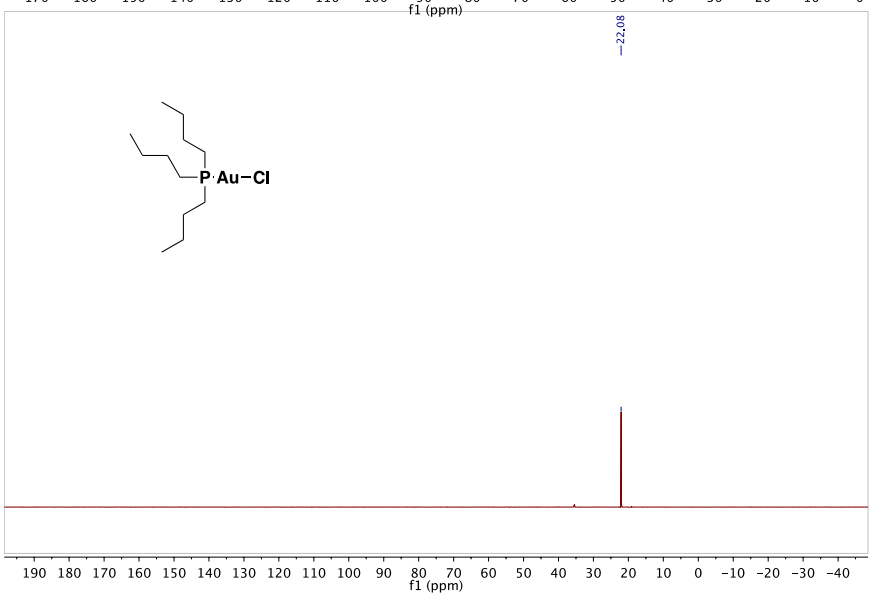
^{1}H NMR ($CDCl_3$, 500 MHz)



^{13}C{^{1}H} NMR ($CDCl_3$, 126 MHz)

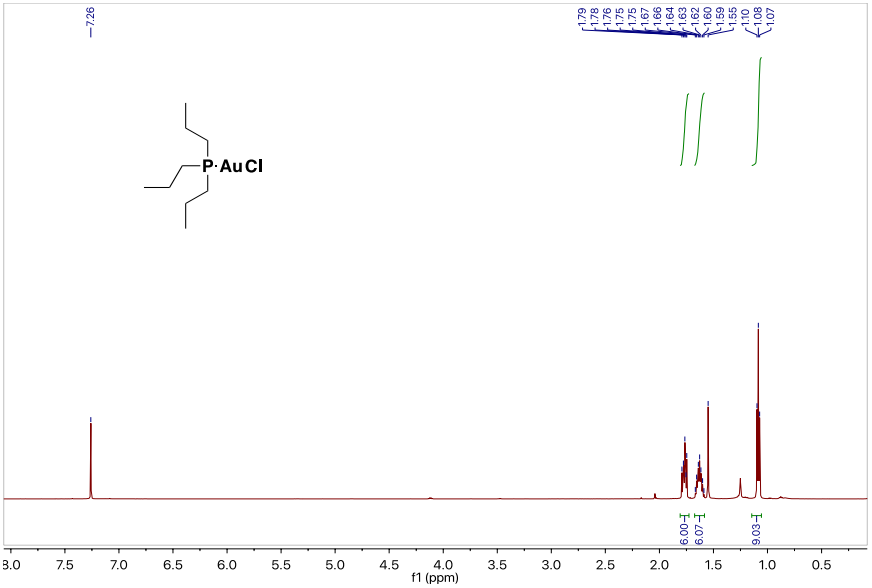


^{31}P{^{1}H} NMR ($CDCl_3$, 202 MHz)

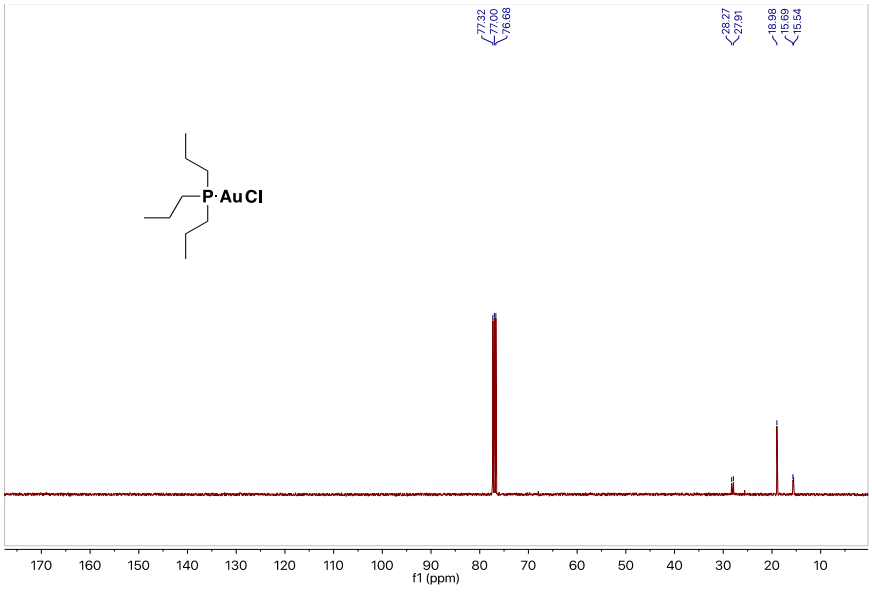


(Tri-*n*-proylphosphine)gold(I) chloride (11)

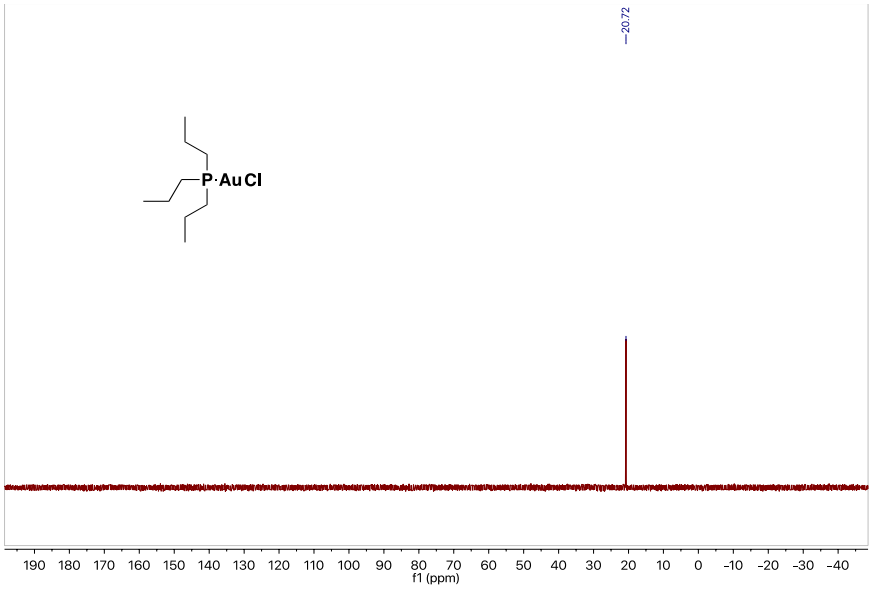
^{1}H NMR ($CDCl_3$, 400 MHz)



^{13}C{^{1}H} NMR ($CDCl_3$, 101 MHz)

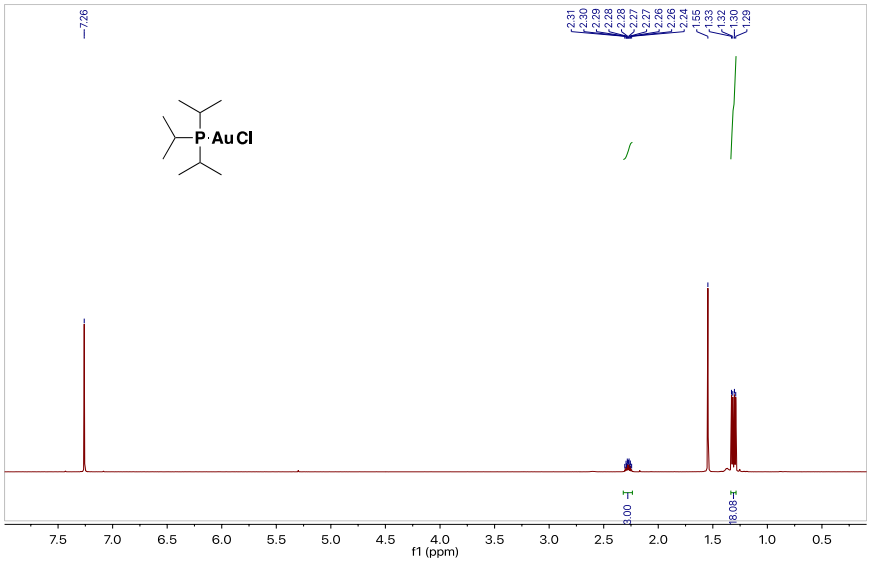


^{31}P{^{1}H} NMR ($CDCl_3$, 202 MHz)

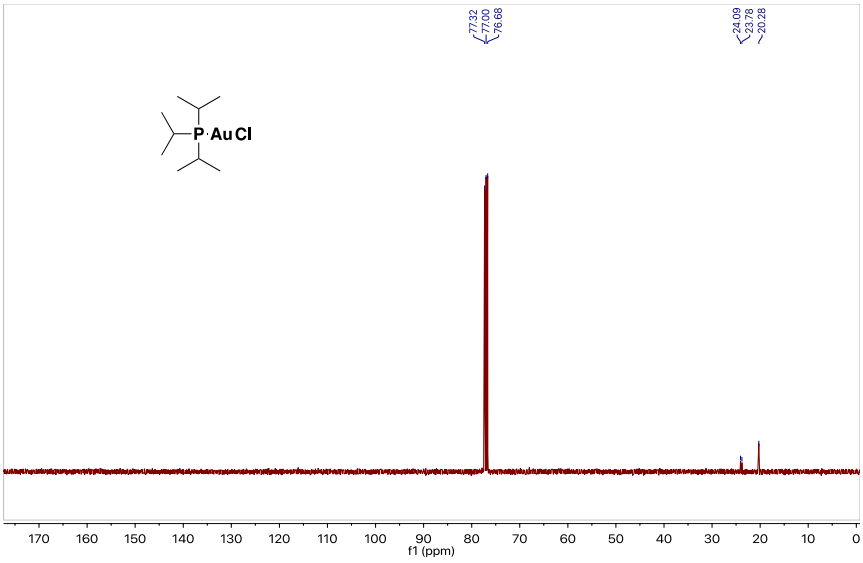


(Triisoproylphosphine)gold(I) chloride (12)

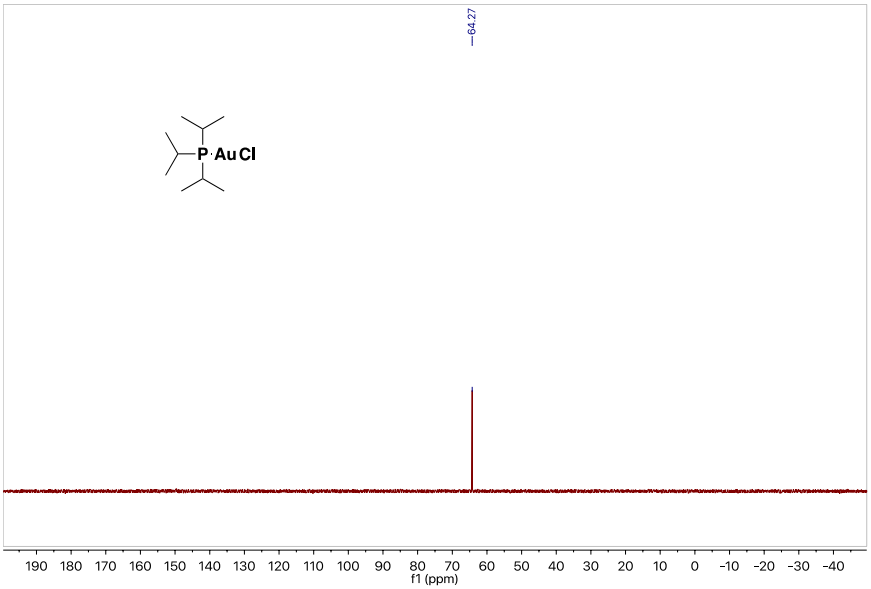
^{1}H NMR ($CDCl_3$, 600 MHz)



^{13}C{^{1}H} NMR ($CDCl_3$, 101 MHz)

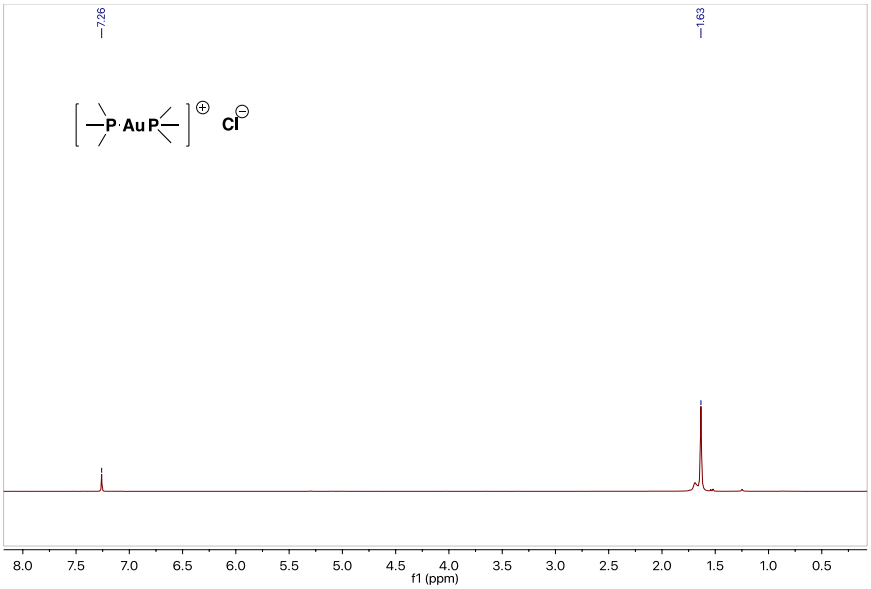


^{31}P{^{1}H} NMR ($CDCl_3$, 162 MHz)

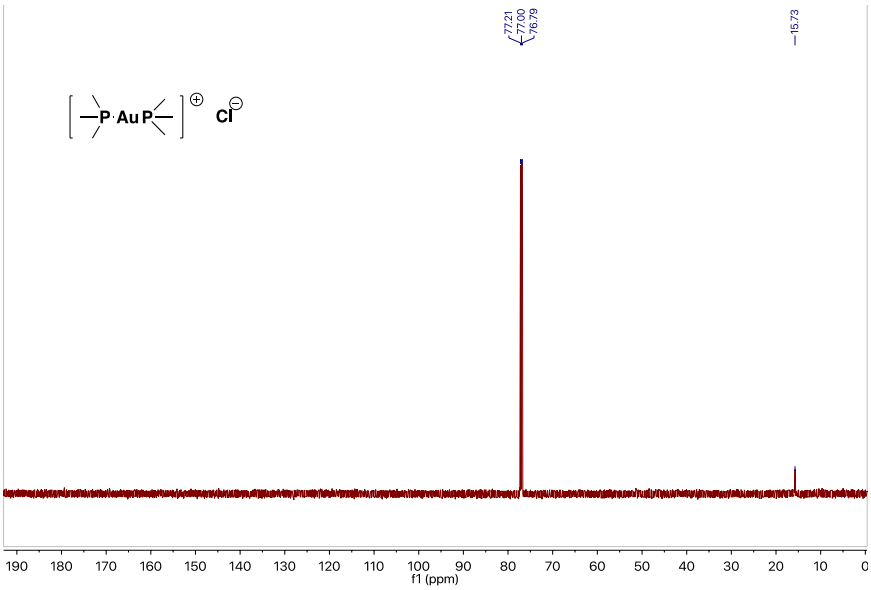


(Trimethylphosphine)gold(I) chloride (13)

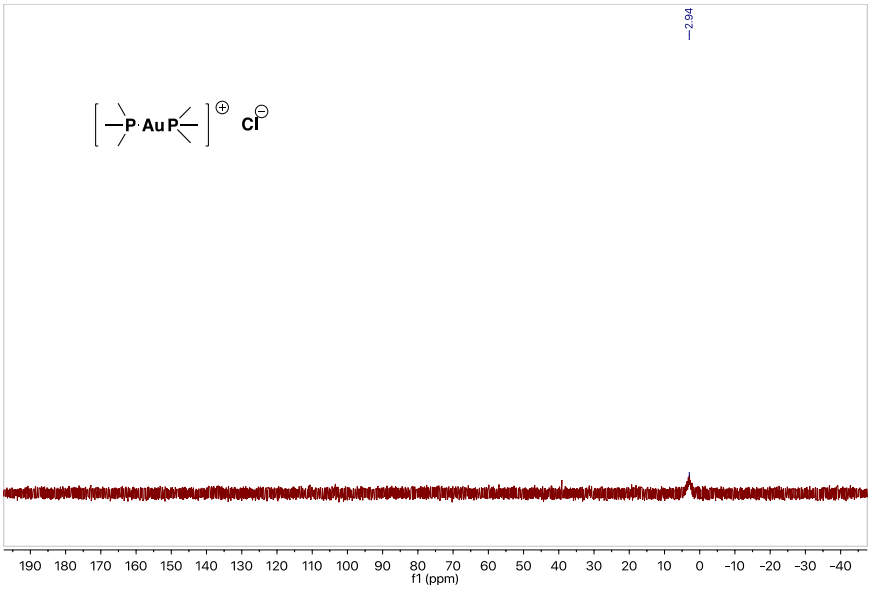
^{1}H NMR ($CDCl_3$, 600 MHz)



^{13}C{^{1}H} NMR ($CDCl_3$, 151 MHz)

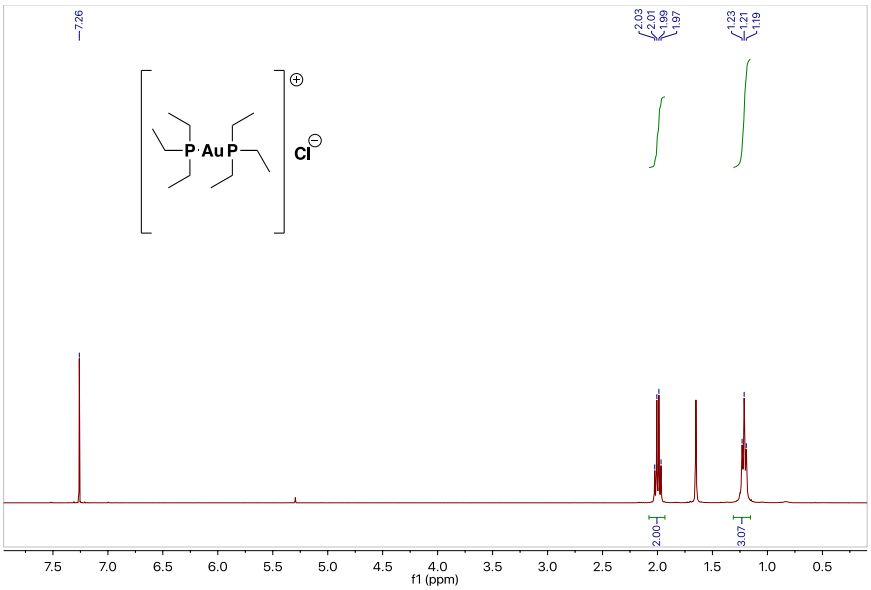


^{31}P{^{1}H} NMR ($CDCl_3$, 243 MHz)

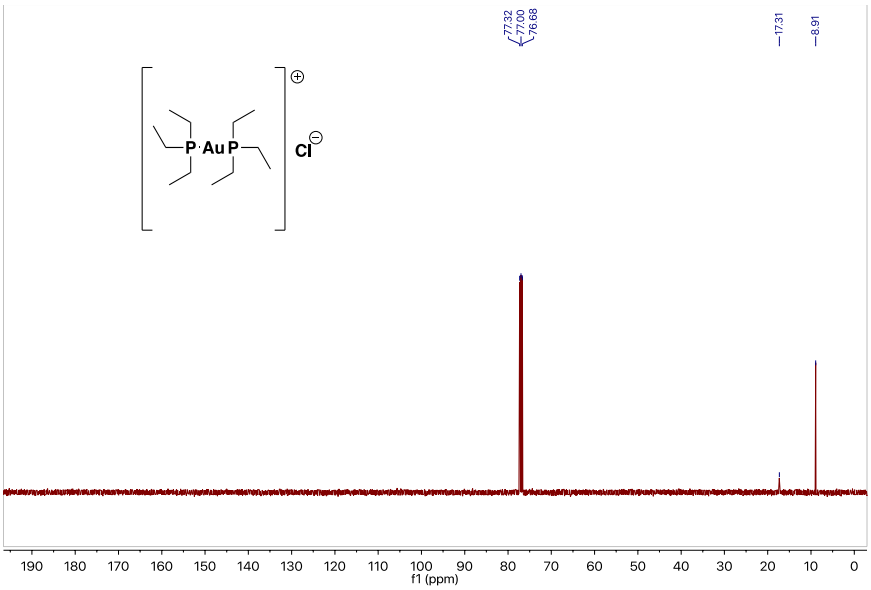


Bis(triethylphosphine)gold(I) chloride (14)

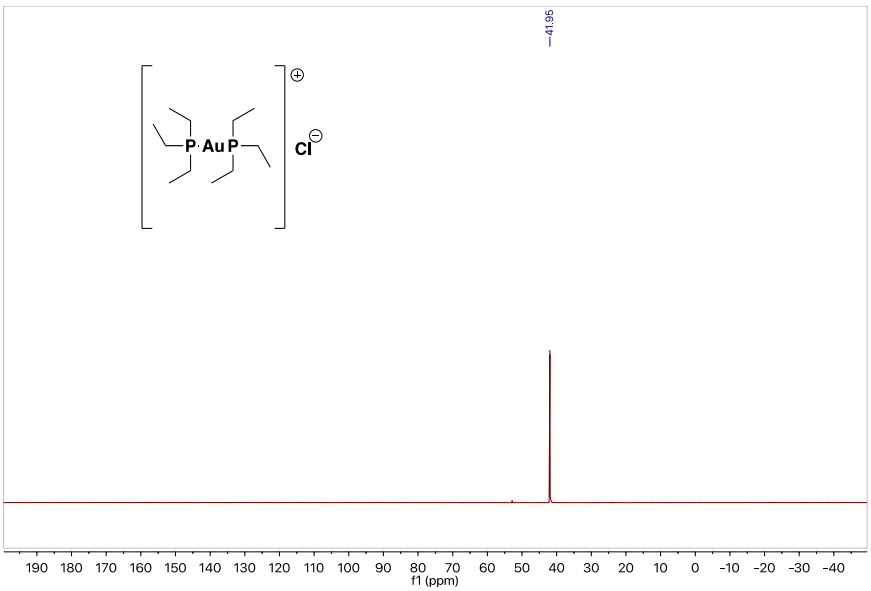
^{1}H NMR ($CDCl_3$, 400 MHz)



$^{13}C\{^{1}H\}$ NMR ($CDCl_3$, 101 MHz)

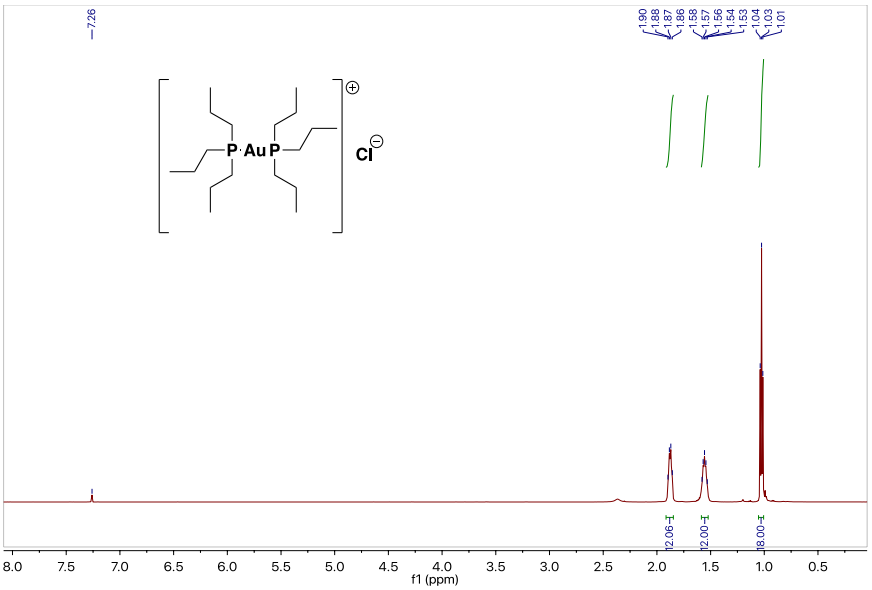


$^{31}P\{^{1}H\}$ NMR ($CDCl_3$, 162 MHz)

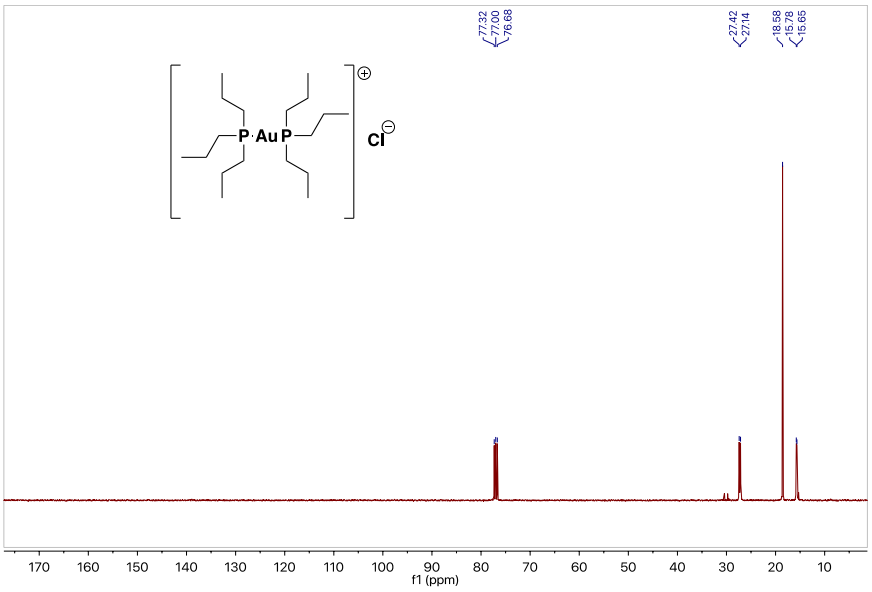


Bis(tri-*n*-propylphosphine)gold(I) chloride (15)

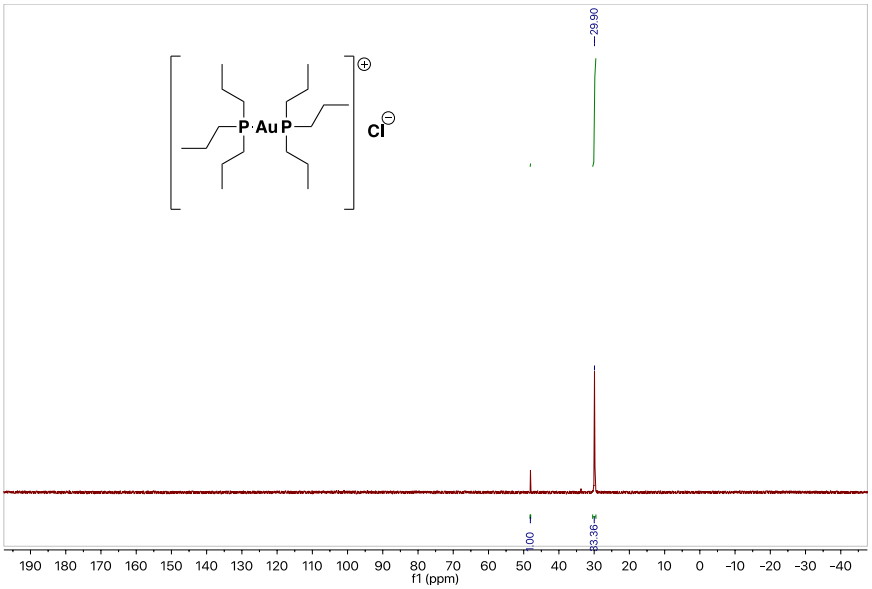
^{1}H NMR ($CDCl_3$, 600 MHz)



^{13}C{^{1}H} NMR ($CDCl_3$, 101 MHz)

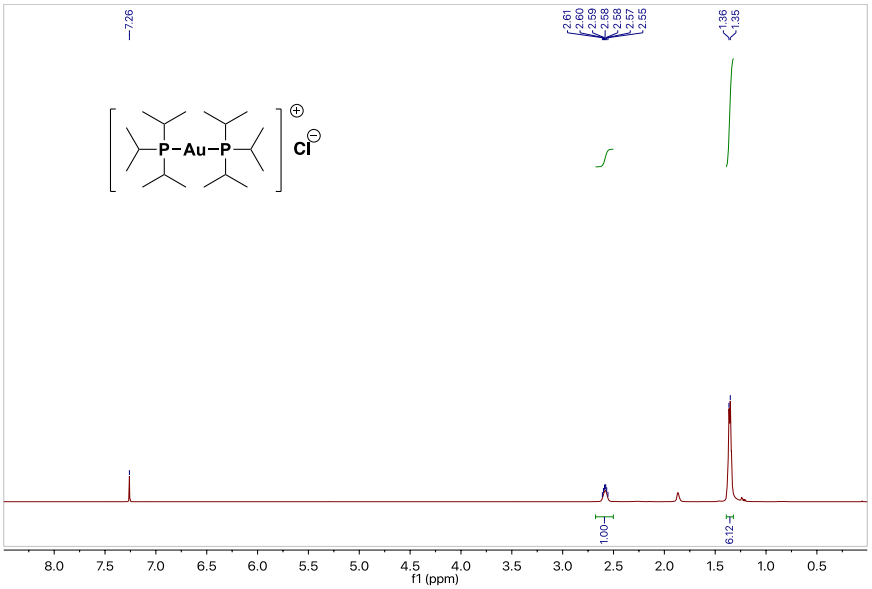


^{31}P{^{1}H} NMR ($CDCl_3$, 243 MHz)

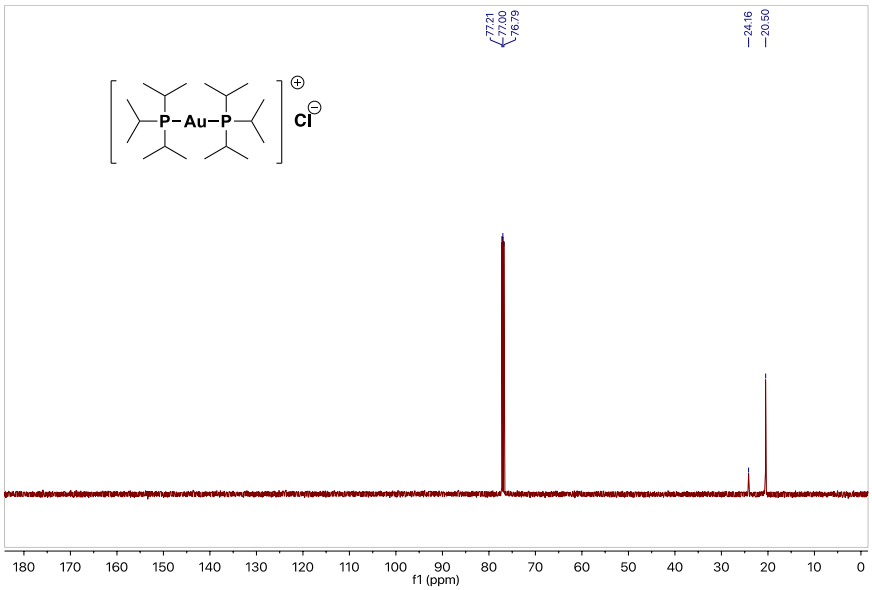


Bis(triisopropylphosphine)gold(I) chloride (16)

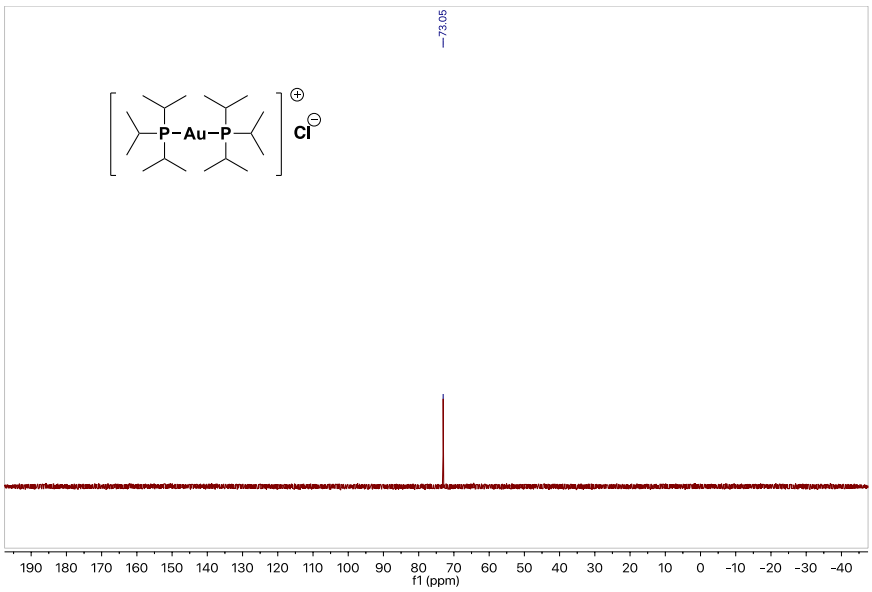
^{1}H NMR ($CDCl_3$, 600 MHz)



$^{13}C\{^{1}H\}$ NMR ($CDCl_3$, 151 MHz)

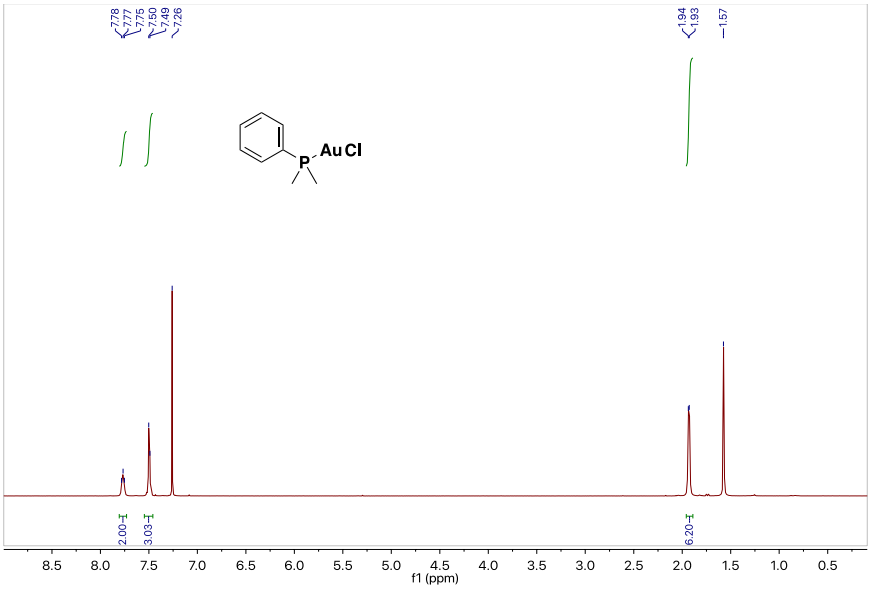


$^{31}P\{^{1}H\}$ NMR ($CDCl_3$, 243 MHz)

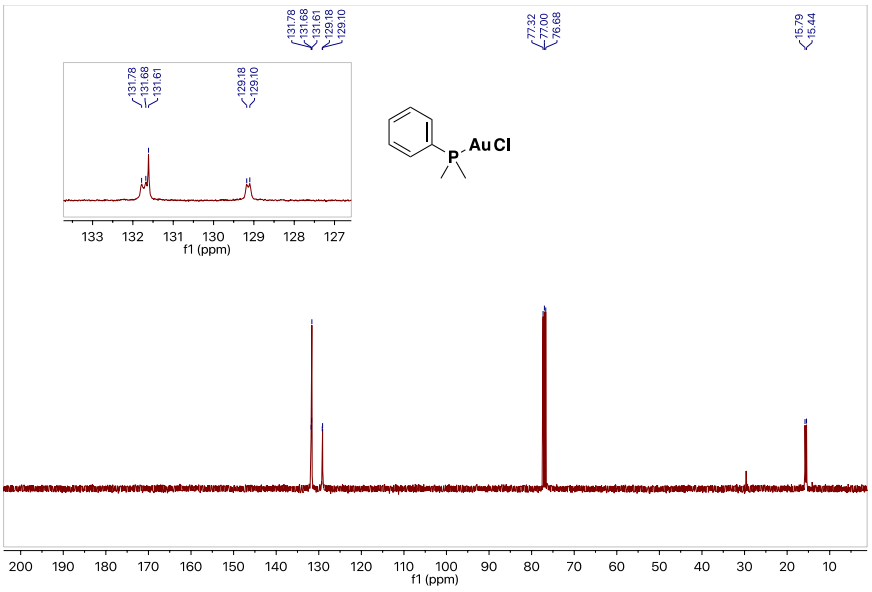


(Dimethylphenylphosphine)gold(I) chloride (18)

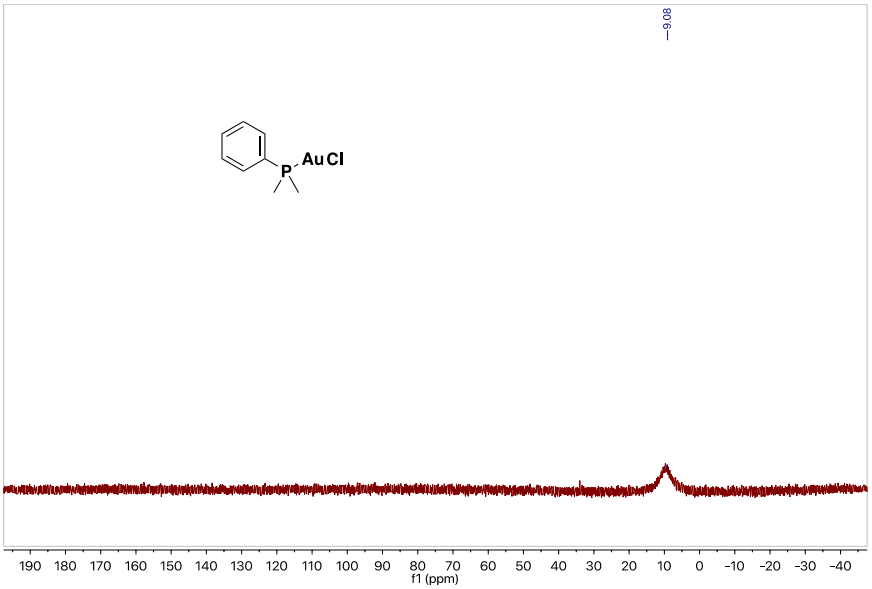
^{1}H NMR ($CDCl_3$, 600 MHz)



^{13}C{^{1}H} NMR ($CDCl_3$, 101 MHz)

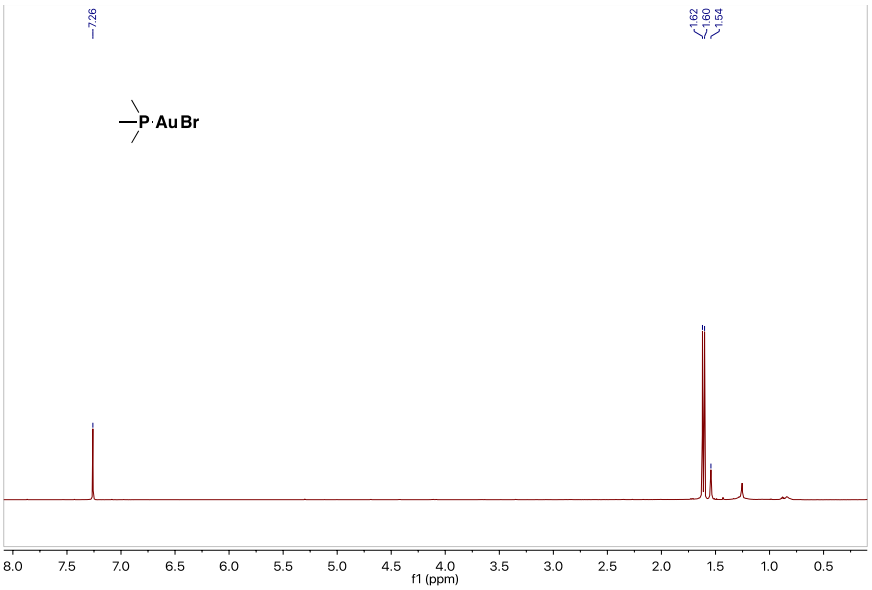


^{31}P{^{1}H} NMR ($CDCl_3$, 243 MHz)

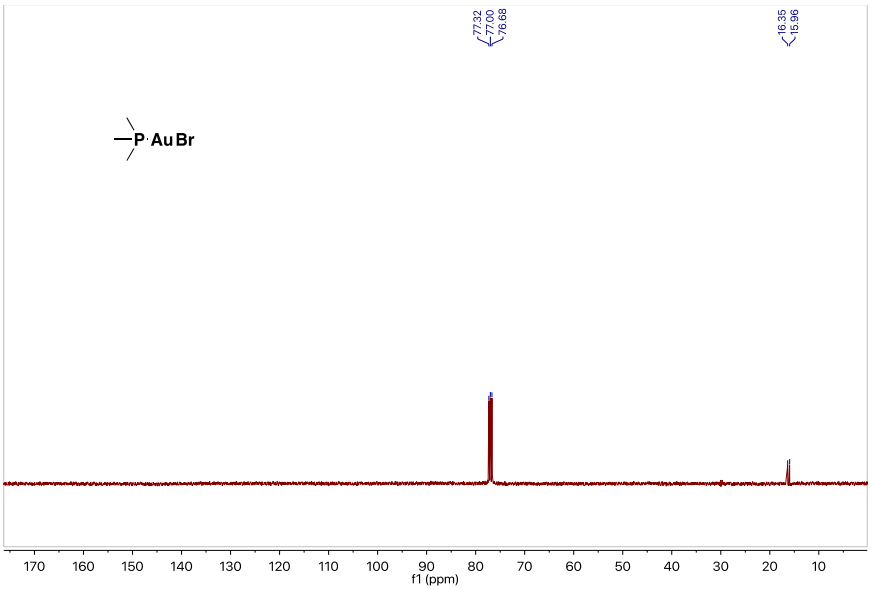


(Trimethylphosphine)gold(I) bromide (23)

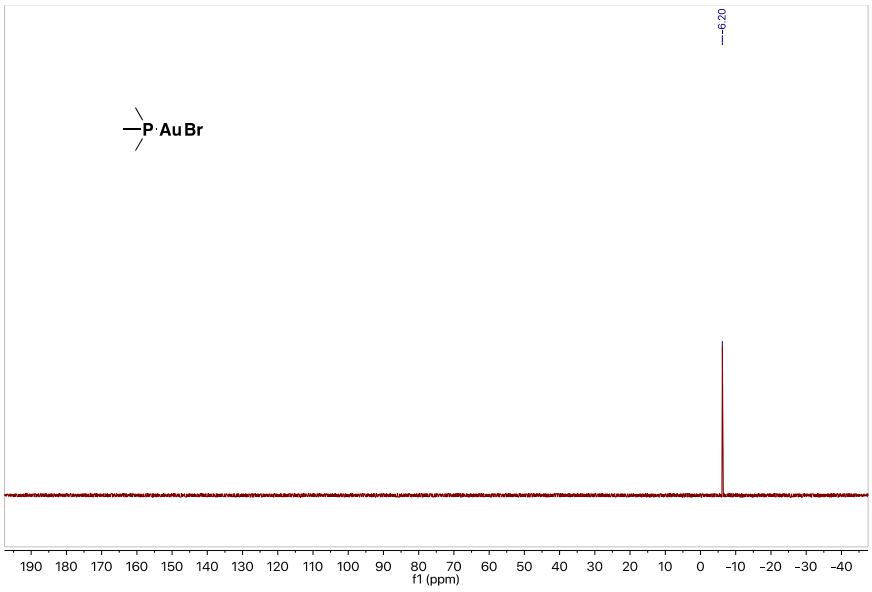
^{1}H NMR ($CDCl_3$, 600 MHz)



^{13}C{^{1}H} NMR ($CDCl_3$, 101 MHz)

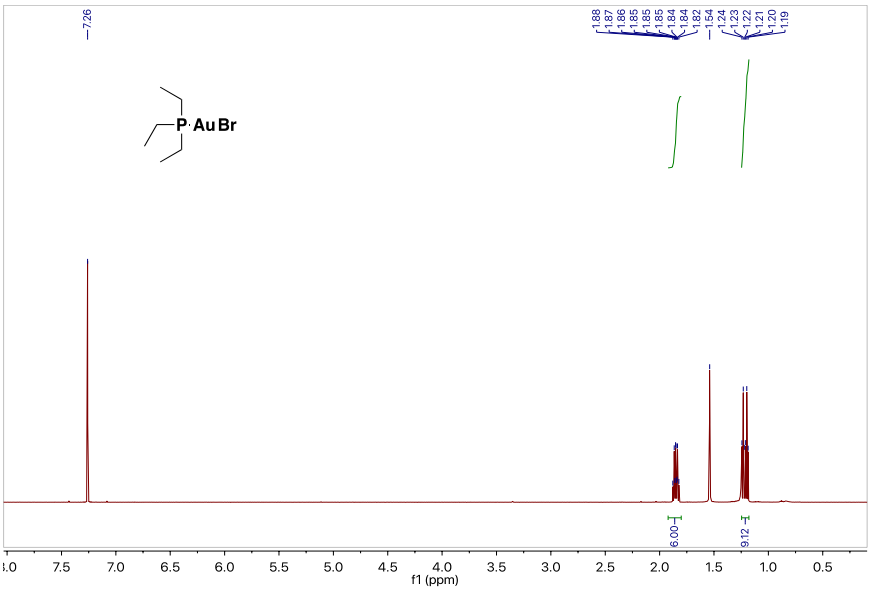


^{31}P{^{1}H} NMR ($CDCl_3$, 243 MHz)

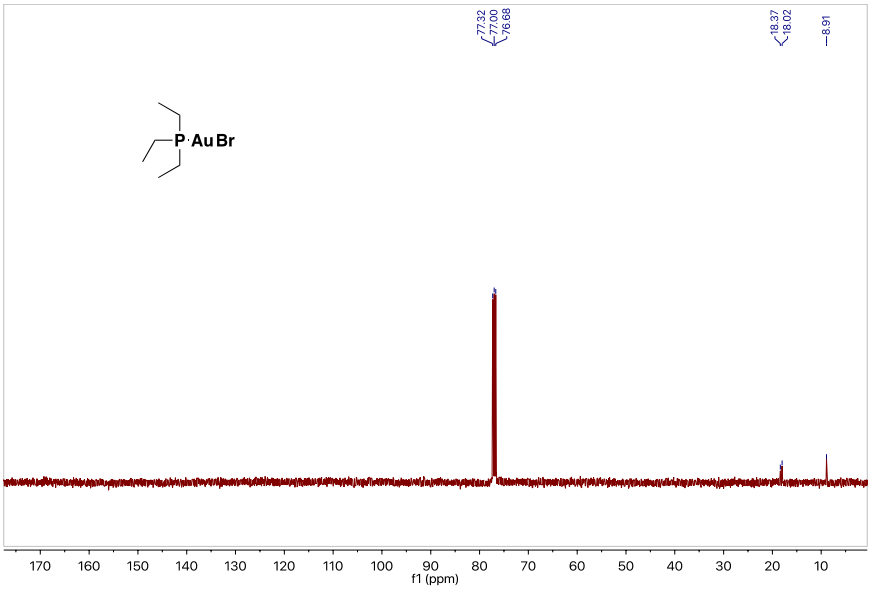


(Triethylphosphine)gold(I) bromide (24)

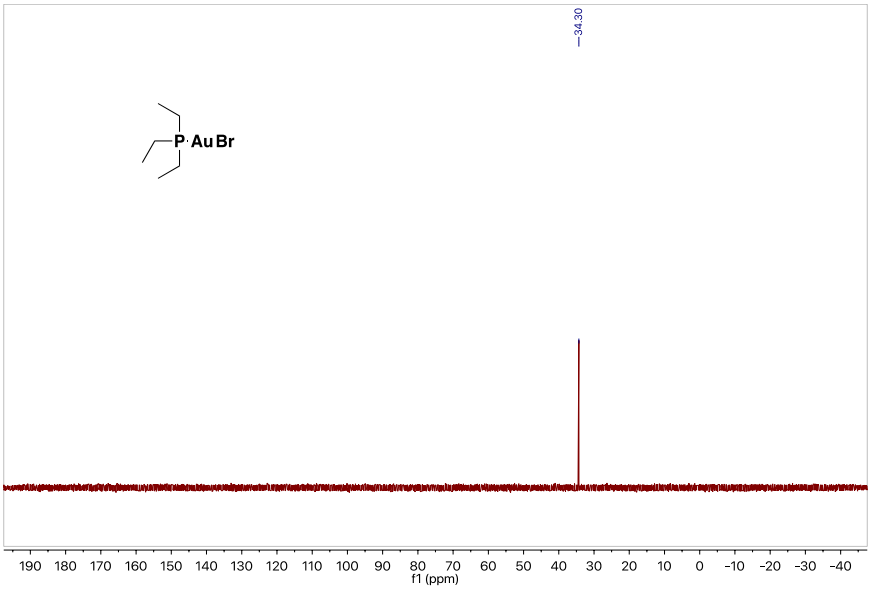
^{1}H NMR ($CDCl_3$, 600 MHz)



^{13}C{^{1}H} NMR ($CDCl_3$, 101 MHz)

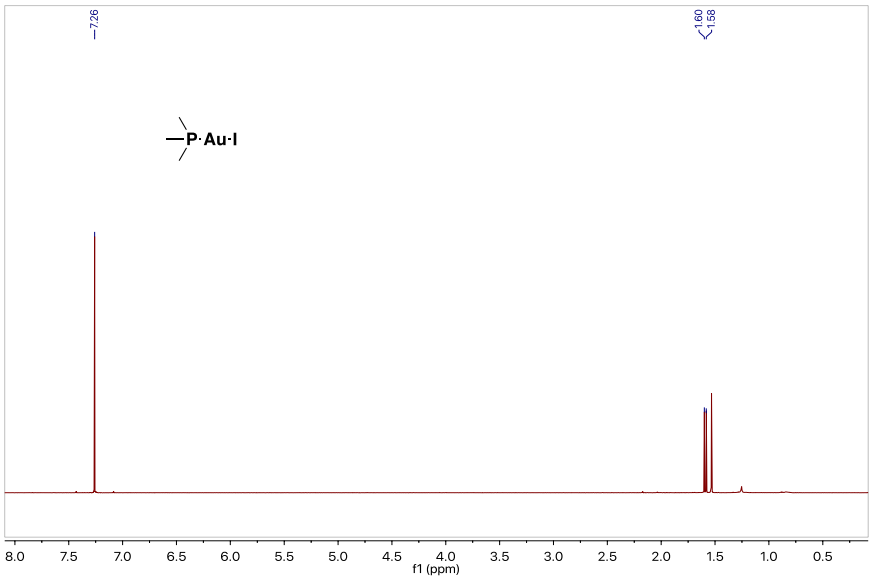


^{31}P{^{1}H} NMR ($CDCl_3$, 243 MHz)

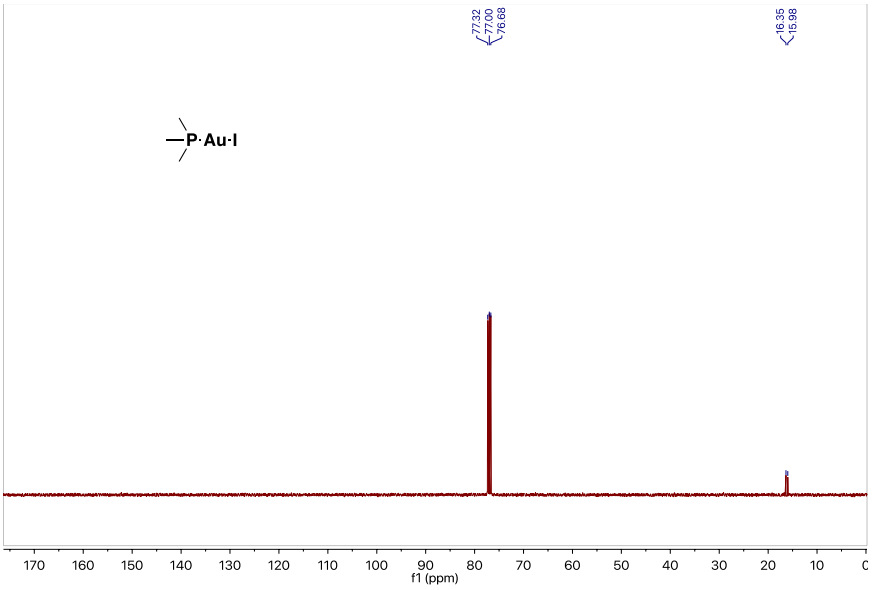


(Trimethylphosphine)gold(I) iodide (25)

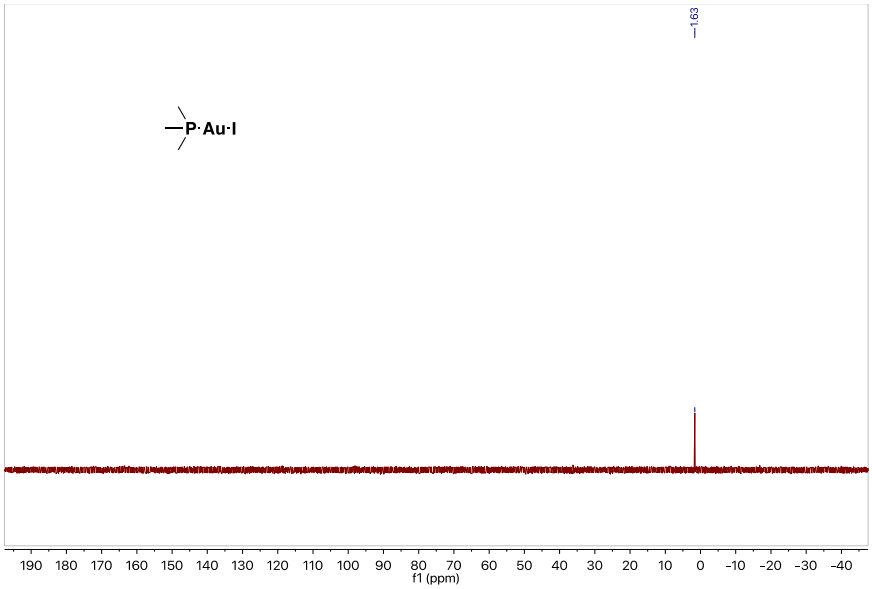
^{1}H NMR ($CDCl_3$, 600 MHz)



^{13}C{^{1}H} NMR ($CDCl_3$, 101 MHz)

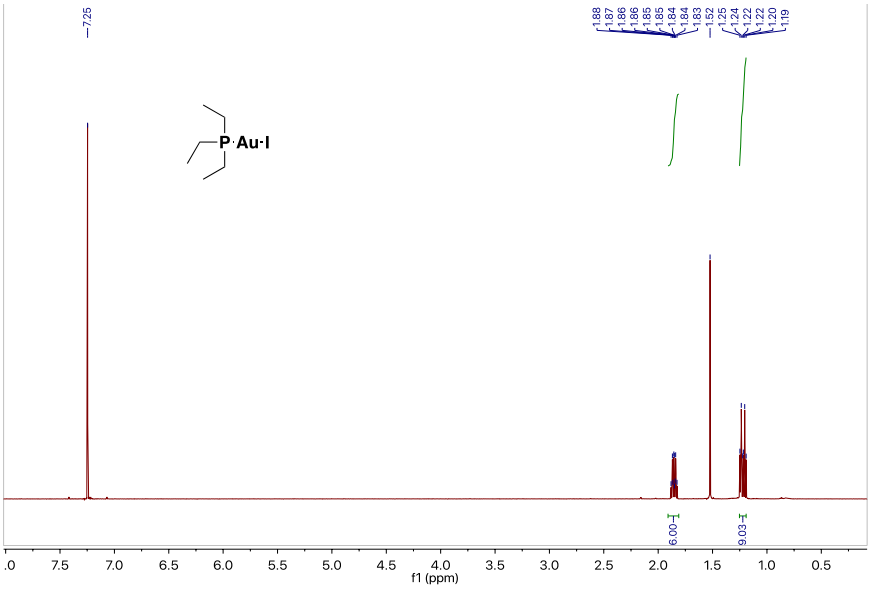


^{31}P{^{1}H} NMR ($CDCl_3$, 243 MHz)

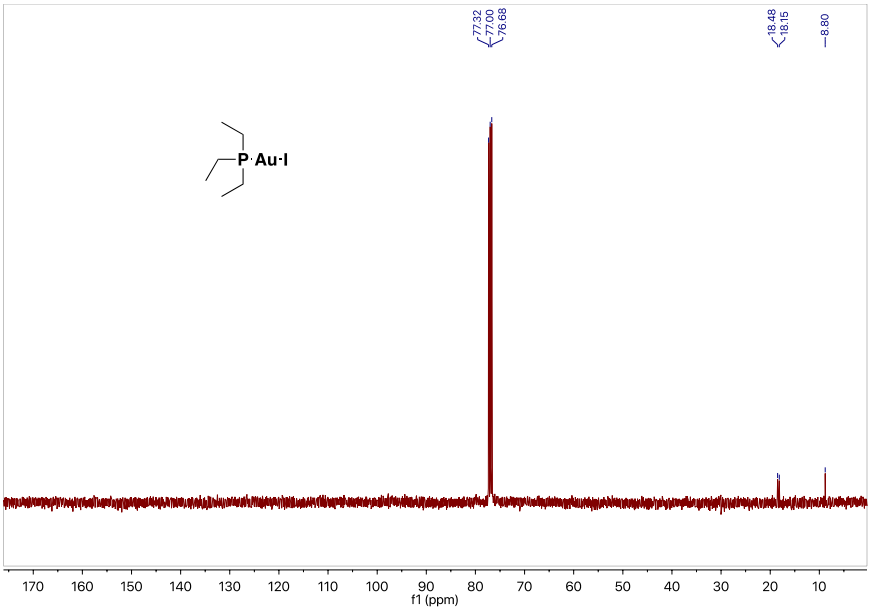


(Triethylphosphine)gold(I) iodide (26)

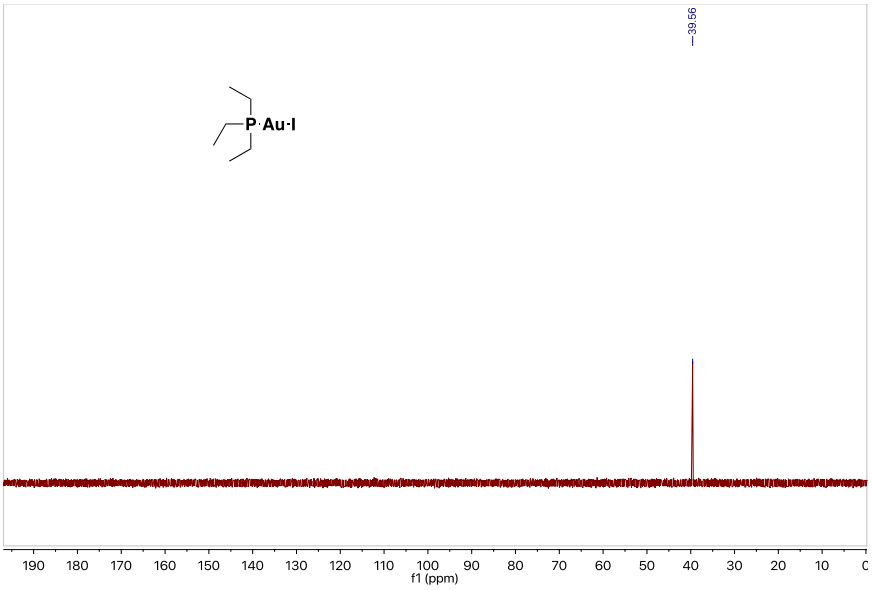
^{1}H NMR ($CDCl_3$, 600 MHz)



^{13}C{^{1}H} NMR ($CDCl_3$, 101 MHz)



^{31}P{^{1}H} NMR ($CDCl_3$, 243 MHz)



PURITY ASSESSMENT BY QUANTITATIVE ^{1}H NMR

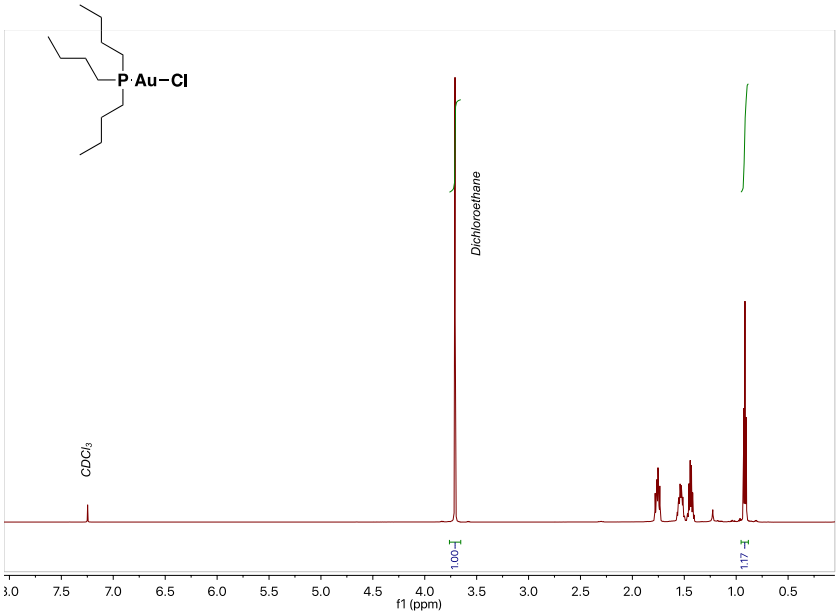
Purity of compounds was determined by absolute quantitative ^{1}H nuclear magnetic resonance (qHNMR) following the "general guidelines for quantitative ^{1}H NMR experiments" provided by the *Journal of Medicinal Chemistry*. Percentage Purity (P [%]) of sample was calculated according to the following equation:

$$P\,[\%] = \frac{n_{IC} \cdot Int_t \cdot MW_t \cdot m_{IC}}{n_t \cdot Int_{IC} \cdot MW_{IC} \cdot m_s} \cdot P_{IC}$$

Where: m_{IC} = mass of internal calibrant (IC)
m_s = mass of sample
Int_{IC} = integral of internal calibrant being used for quantification
Int_t = integral of target analyte being used for quantification
n_{IC} = number of protons that give rise to Int_{IC}
n_t = number of protons that give rise to Int_t
MW_{IC} = molecular weight of the internal calibrant
MW_t = molecular weight of the target analyte
P_{IC} = purity of the internal calibrant

The internal calibrant used for qHNMR experiments was 1,2-dichloroethane (Acros Organics), molecular weight (MW_{IC}) = 98.96 g/mol. Purity of the internal standard (P_{IC}) was 99.8 % according to the chemical specifications. Ten μL (density = 1.25 g/mL, m_{IC} = 12.5 mg) of internal calibrant was added to the qHNMR samples using a micropipette.

qHNMR of (Tri-*n*-butylphosphine)gold(I) chloride (9)
($CDCl_3$, 600 MHz)



m_s = 29.6 mg, m_{IC} = 12.5 mg

P_{IC} = 99.8 %

Int_t = 1.17, n_t = 9

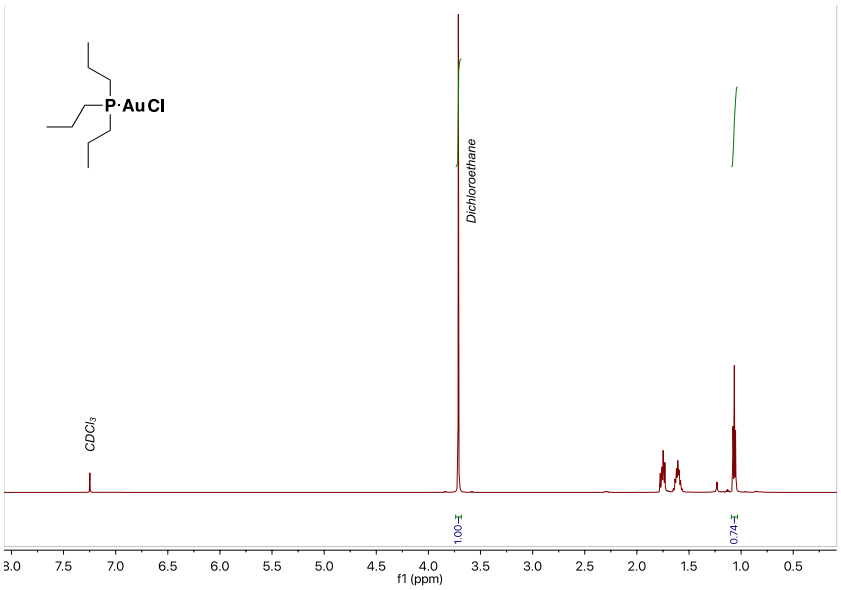
Int_{IC} = 1, n_{IC} = 4

MW_t = 434.73 g/mol

MW_{IC} = 98.96 g/mol

P **[%]** = 96.27 %

qHNMR of (Tri-*n*-propylphosphine)gold(I) chloride (11)
($CDCl_3$, 600 MHz)



m_s = 16.4 mg, m_{IC} = 12.5 mg

P_{IC} = 99.8 %

Int_t = 0.74, n_t = 9

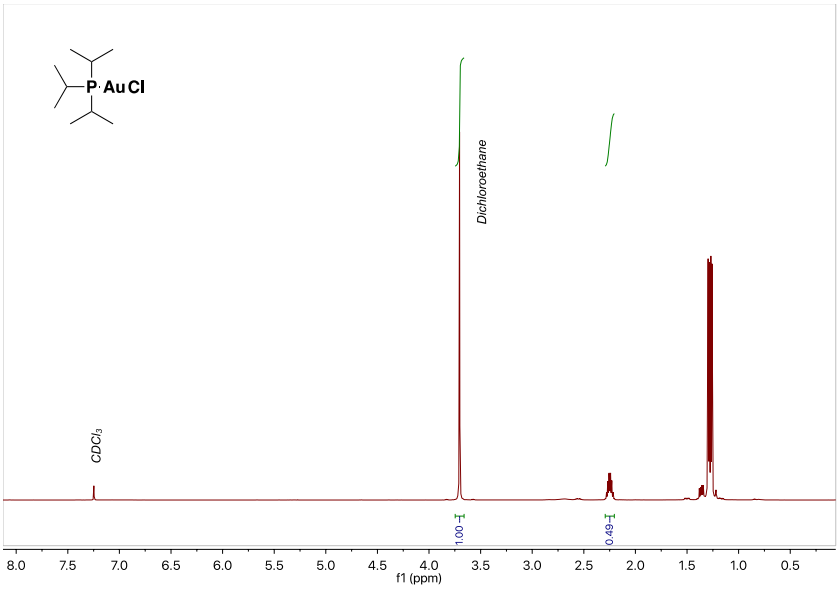
Int_{IC} = 1, n_{IC} = 4

MW_t = 392.65 g/mol

MW_{IC} = 98.96 g/mol

P **[%]** = 99.26 %

qHNMR of (Triisopropylphosphine)gold(I) chloride (12)
($CDCl_3$, 600 MHz)



m_s = 33.6 mg, m_{IC} = 12.5 mg

P_{IC} = 99.8 %

Int_t = 0.49, n_t = 3

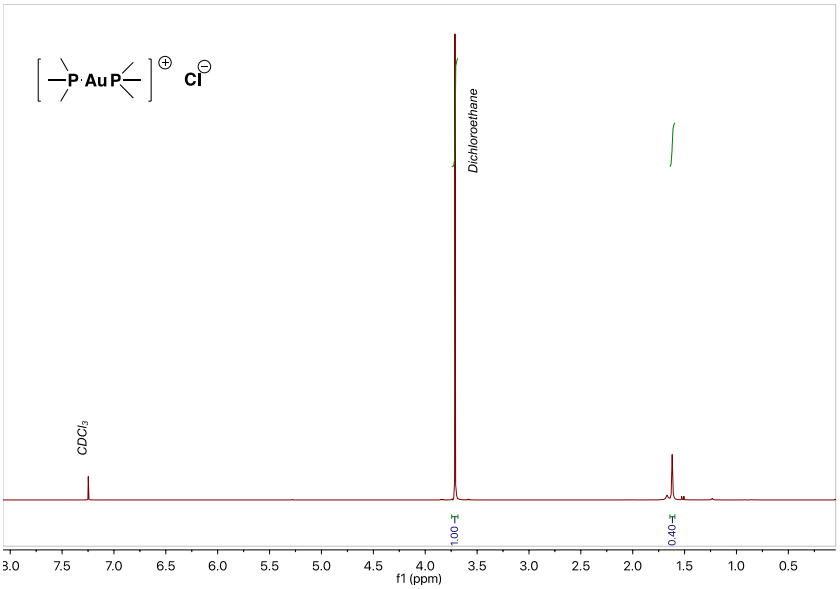
Int_{IC} = 1, n_{IC} = 4

MW_t = 392.65 g/mol

MW_{IC} = 98.96 g/mol

P [%] = 96.24 %

qHNMR of Bis(trimethylphosphine)gold(I) chloride (13)
($CDCl_3$, 600 MHz)



m_s = 4.5 mg, m_{IC} = 12.5 mg

P_{IC} = 99.8 %

Int_t = 0.40, n_t = 18

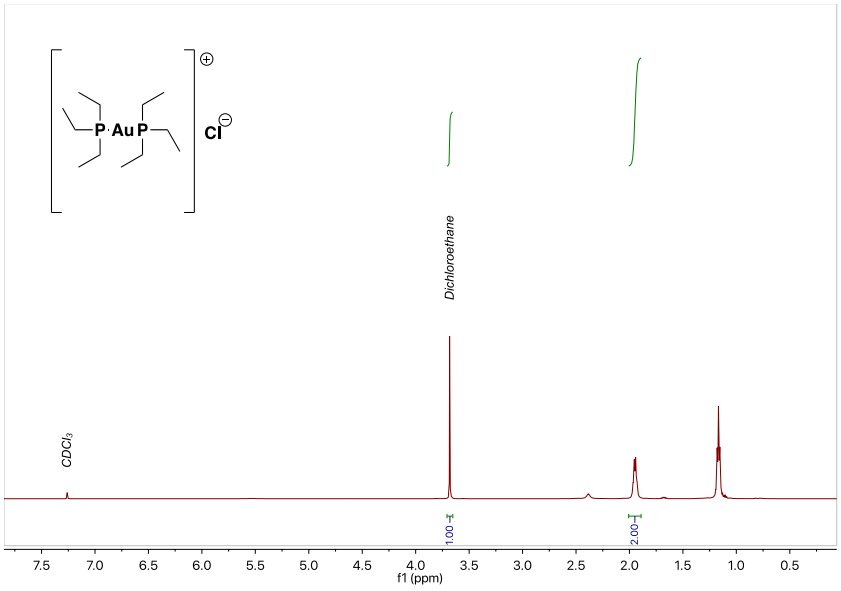
Int_{IC} = 1, n_{IC} = 4

MW_t = 384.57 g/mol

MW_{IC} = 98.96 g/mol

P [%] = 95.76 %

qHNMR of Bis(triethylphosphine)gold(I) chloride (14)
($CDCl_3$, 600 MHz)



m_s = 40.4 mg, m_{IC} = 12.5 mg

P_{IC} = 99.8 %

Int_t = 2, n_t = 12

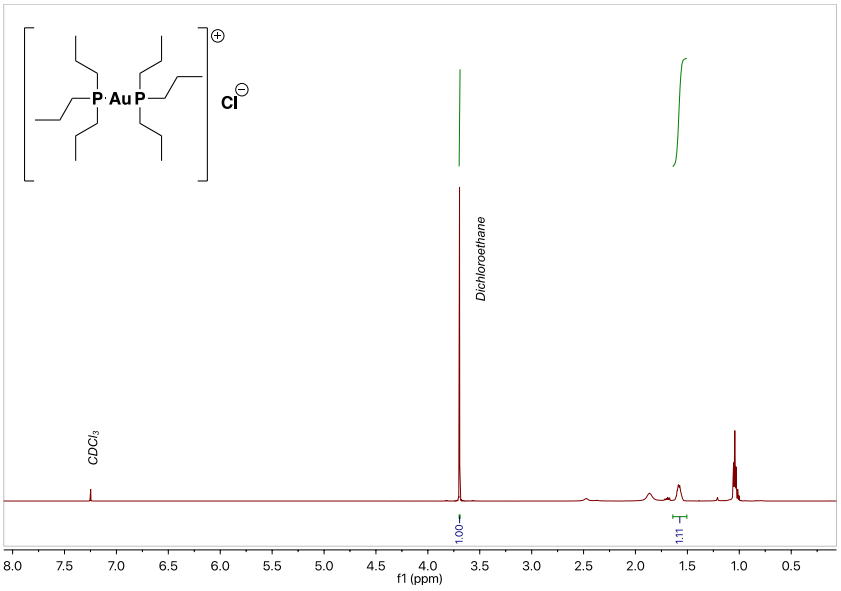
Int_{IC} = 1, n_{IC} = 4

MW_t = 468.73 g/mol

MW_{IC} = 98.96 g/mol

P [%] = 97.50 %

qHNMR of Bis(tripropylphosphine)gold(I) chloride (15)
($CDCl_3$, 600 MHz)



m_s = 27.1 mg, m_{IC} = 12.5 mg,

P_{IC} = 99.8 %

Int_t = 1.11, n_t = 12

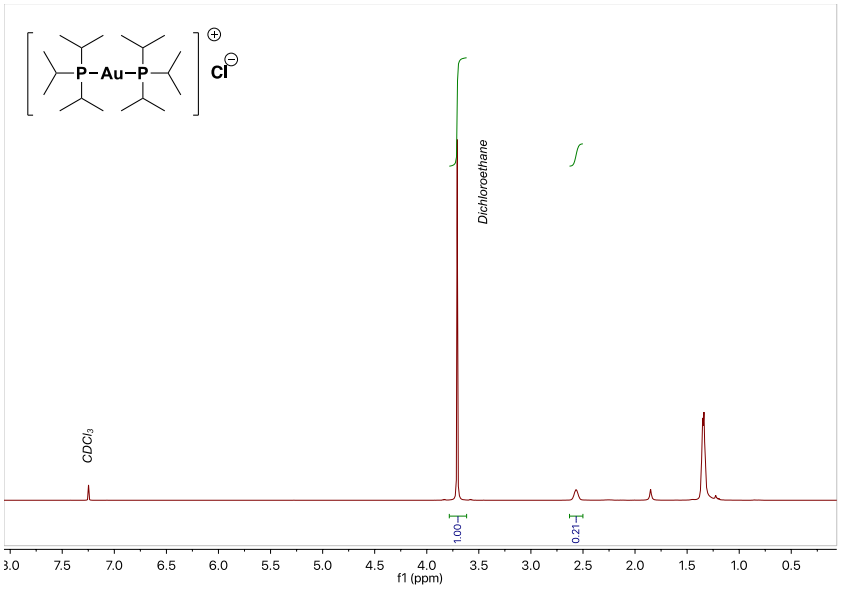
Int_{IC} = 1, n_{IC} = 4

MW_t = 552.89 g/mol

MW_{IC} = 98.96 g/mol

P [%] = 95.15 %

qHNMR of Bis(triisopropylphosphine)gold(I) chloride (16)
($CDCl_3$, 600 MHz)



m_s = 10.1 mg, m_{IC} = 12.5 mg

P_{IC} = 99.8 %

Int_t = 0.21, n_t = 6

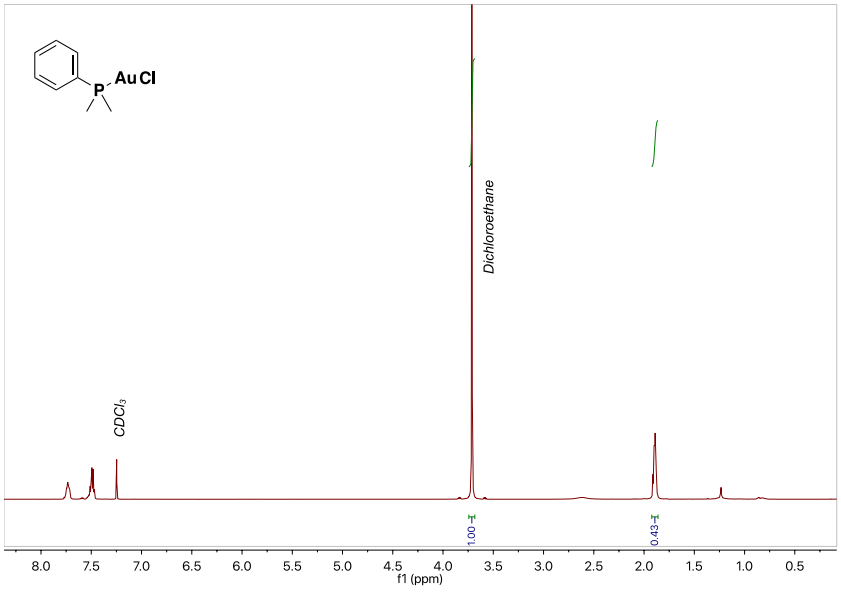
Int_{IC} = 1, n_{IC} = 4

MW_t = 552.89 g/mol

MW_{IC} = 98.96 g/mol

P **[%]** = 96.61 %

qHNMR of (Dimethylphenylphosphine)gold(I) chloride (18)
($CDCl_3$, 600 MHz)



m_s = 13.8 mg, m_{IC} = 12.5 mg

P_{IC} = 99.8 %

Int_t = 0.43, n_t = 6

Int_{IC} = 1, n_{IC} = 4

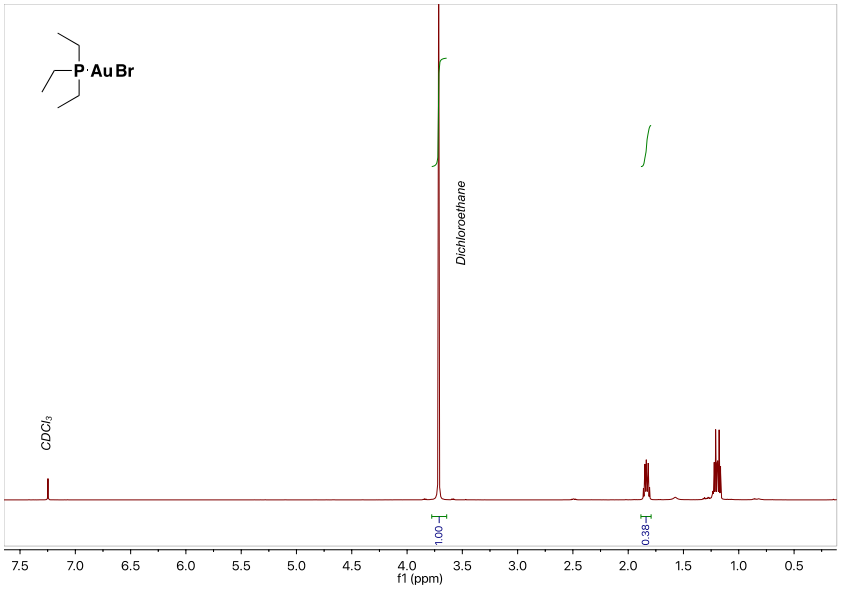
MW_t = 370.56 g/mol

MW_{IC} = 98.96 g/mol

P **[%]** = 97.03 %

qHNMR of (Triethylphosphine)gold(I) bromide (24)

($CDCl_3$, 600 MHz)



m_s = 12.8 mg, m_{IC} = 12.5 mg

P_{IC} = 99.8 %

Int_t = 0.38, n_t = 6

Int_{IC} = 1, n_{IC} = 4

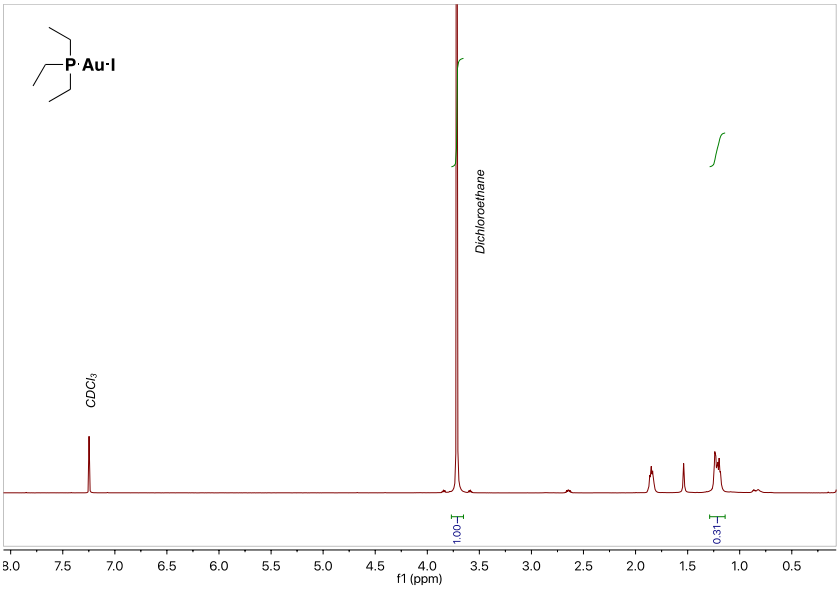
MW_t = 395.03 g/mol

MW_{IC} = 98.96 g/mol

P [%] = 98.55 %

qHNMR of (Triethylphosphine)gold(I) iodide (26)

($CDCl_3$, 600 MHz)



m_s = 7.9 mg, m_{IC} = 12.5 mg

P_{IC} = 99.8 %

Int_t = 0.31, n_t = 9

Int_{IC} = 1, n_{IC} = 4

MW_t = 442.03 g/mol

MW_{IC} = 98.96 g/mol

P [%] = 97.18 %