Highly active group 11 metal complexes with α-hydrazidophosphonate ligands

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Table of contents

1. Characterization of complexes 1-14

1.11. Spectra of complex $[Ag(L1)_2]OTf$ (1)

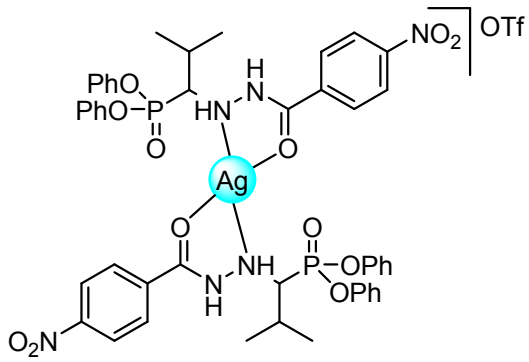


Figure S1. ^{1}H NMR spectrum of compound **$[Ag(L1)_2]OTf$ (1)**

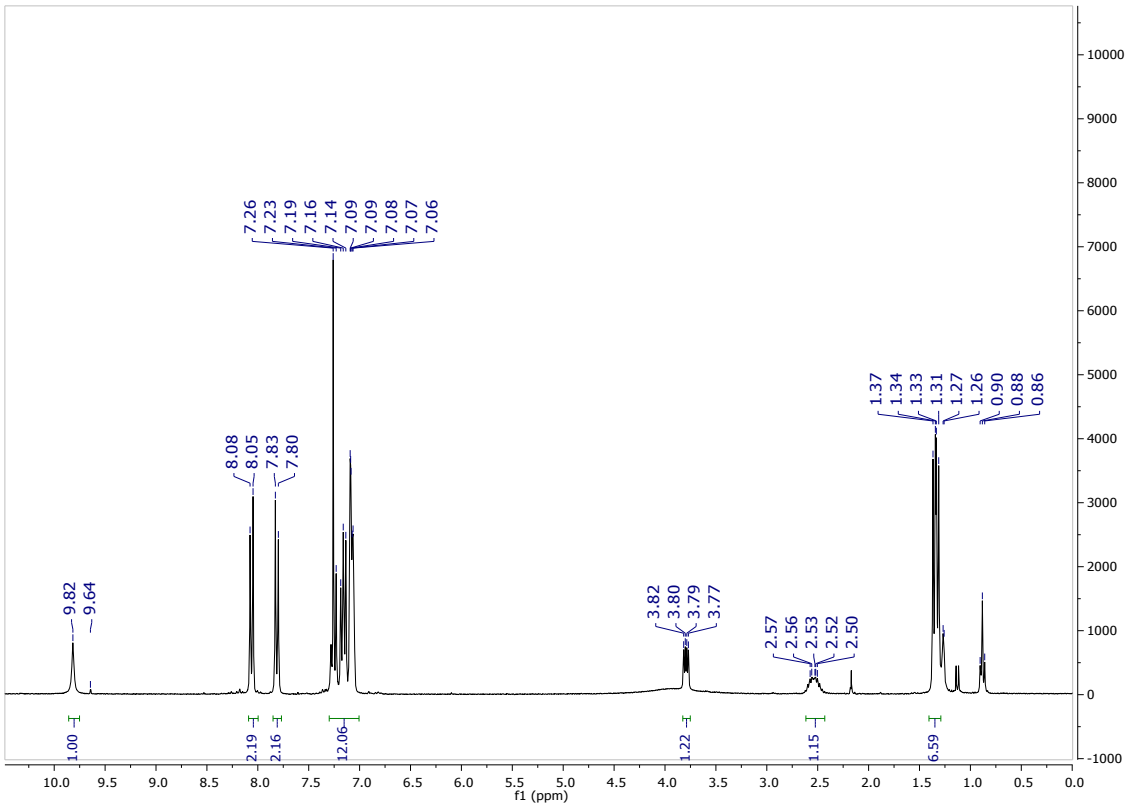


Figure S2. ^{31}P NMR spectrum of compound **$[Ag(L1)_2]OTf$ (1)**

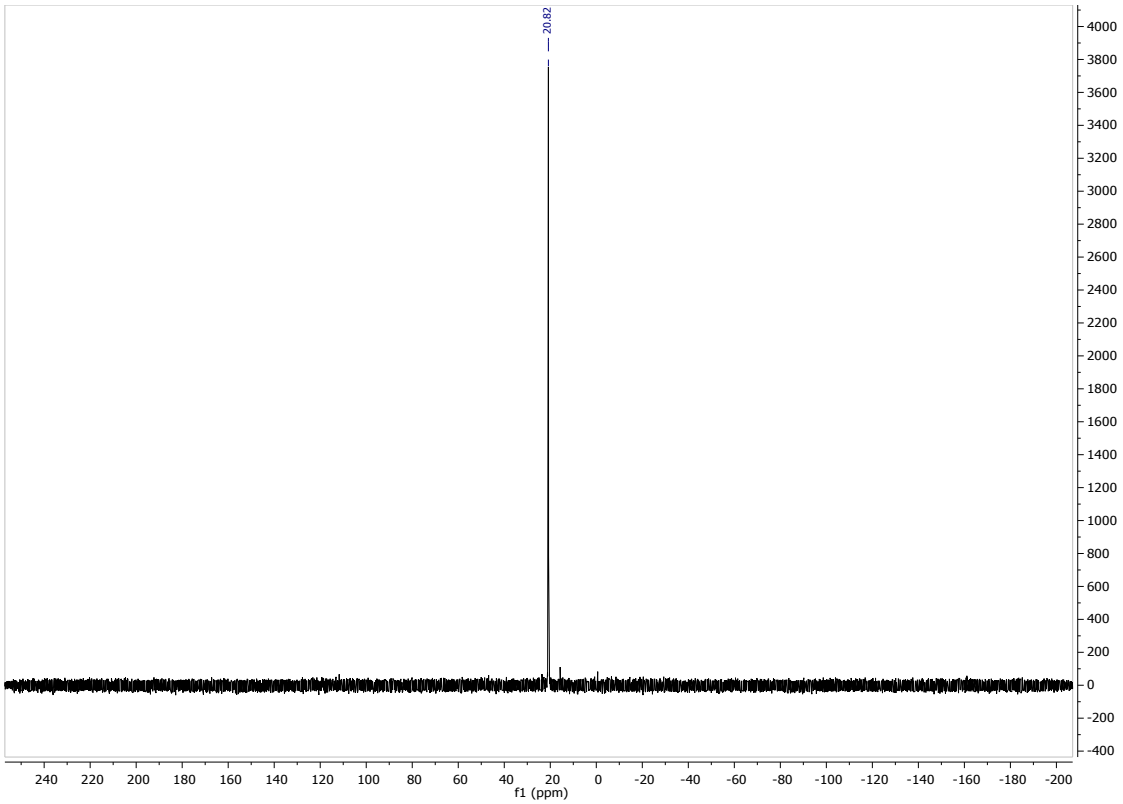
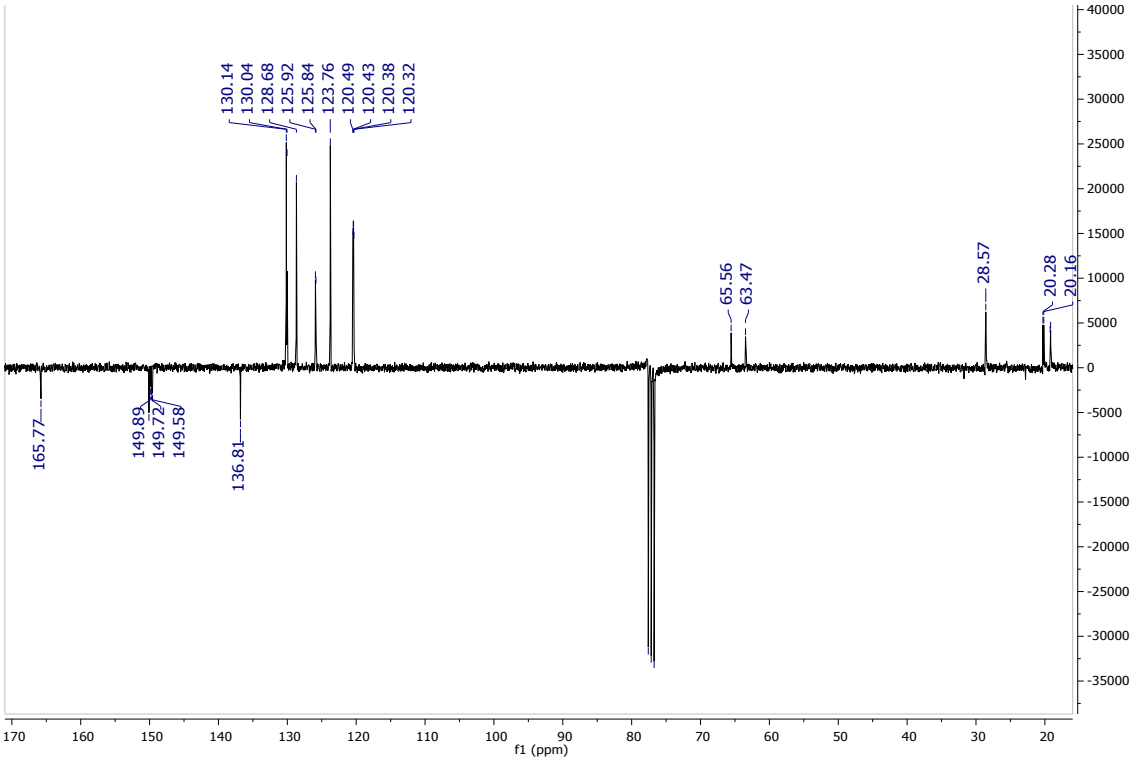


Figure S3. ^{13}C-APT NMR spectrum of compound **[Ag(L1)$_2$]OTf (1)**



1.2. Spectra of complex $[Ag(L2)_2]OTf$ (2)

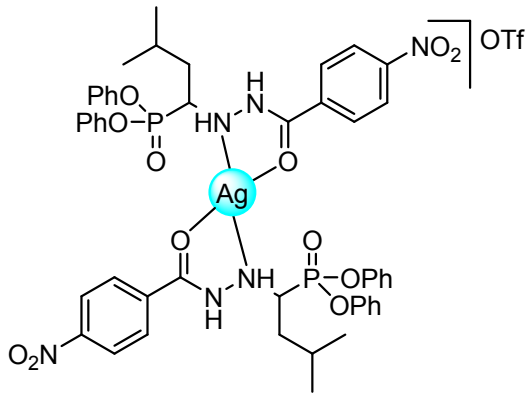


Figure S4. ^1H NMR spectrum of compound **$[Ag(L2)_2]OTf$ (2)**

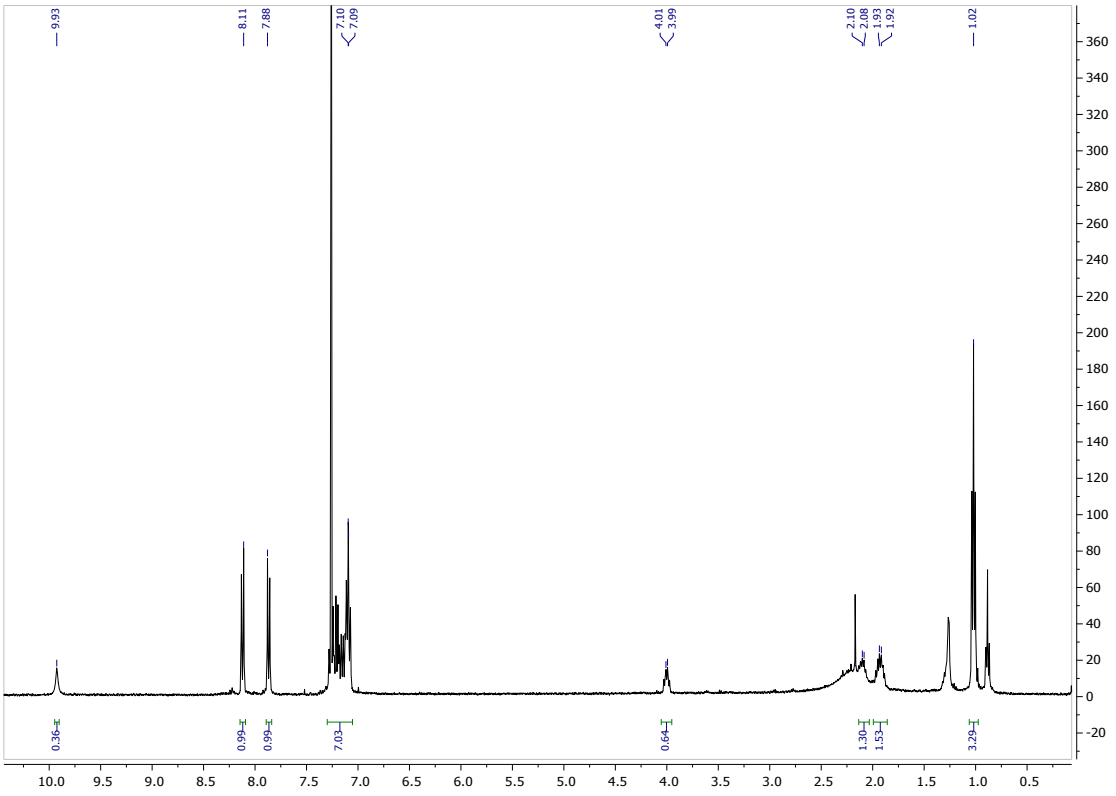


Figure S5. ^{31}P NMR spectrum of compound **[Ag(L2)$_2$]OTf (2)**

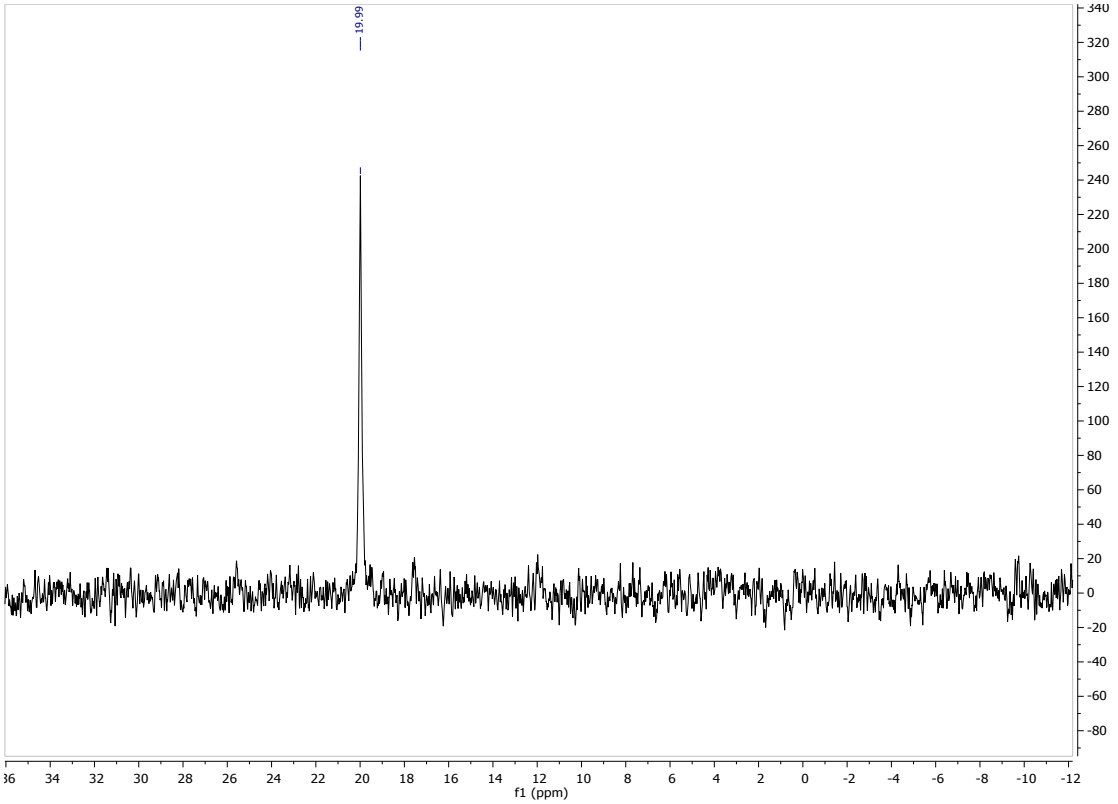
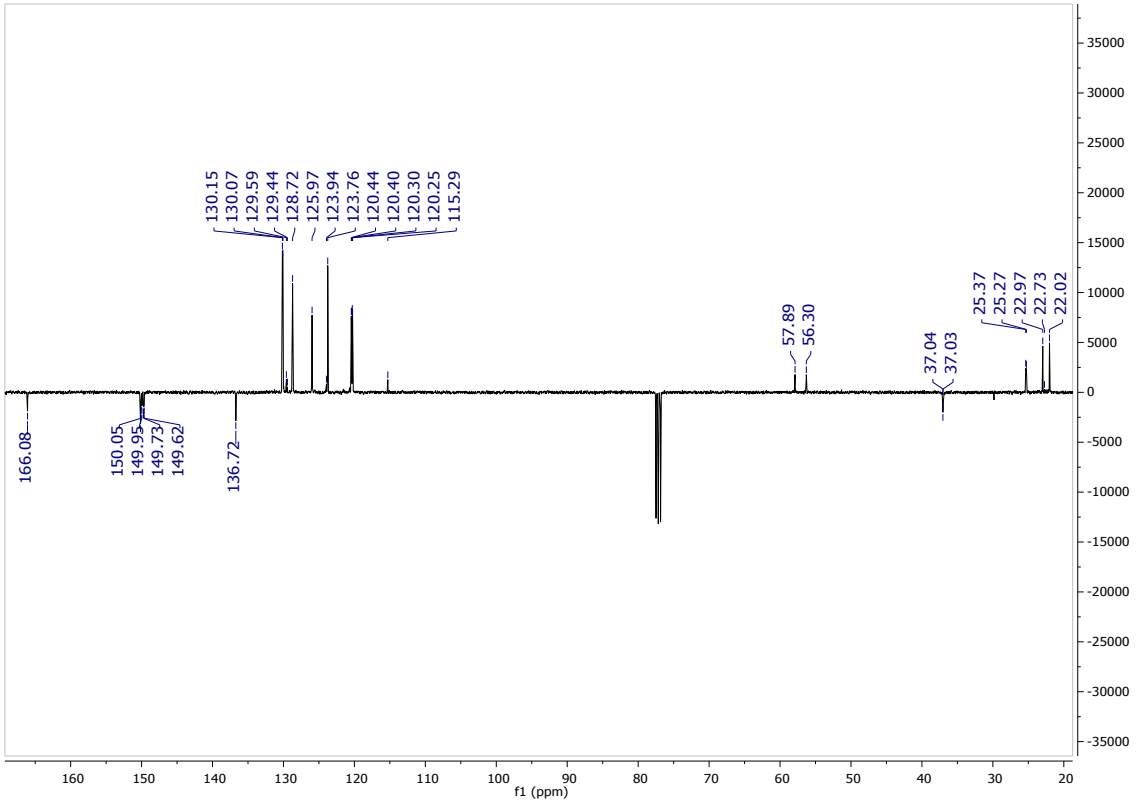


Figure S6. ^{13}C-APT spectrum of compound **[Ag(L2)$_2$]OTf (2)**



1.3. Spectra of complex $[Ag(L3)_2]OTf$ (3)

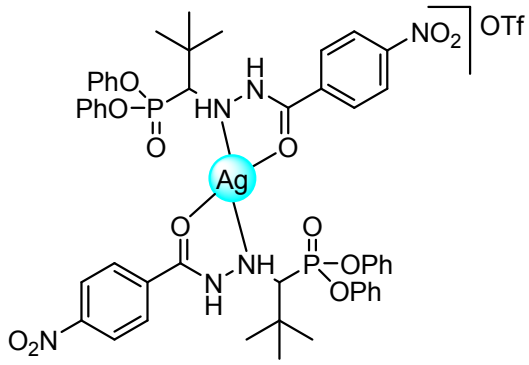


Figure S7. ^{1}H NMR spectrum of compound **$[Ag(L3)_2]OTf$ (3)**

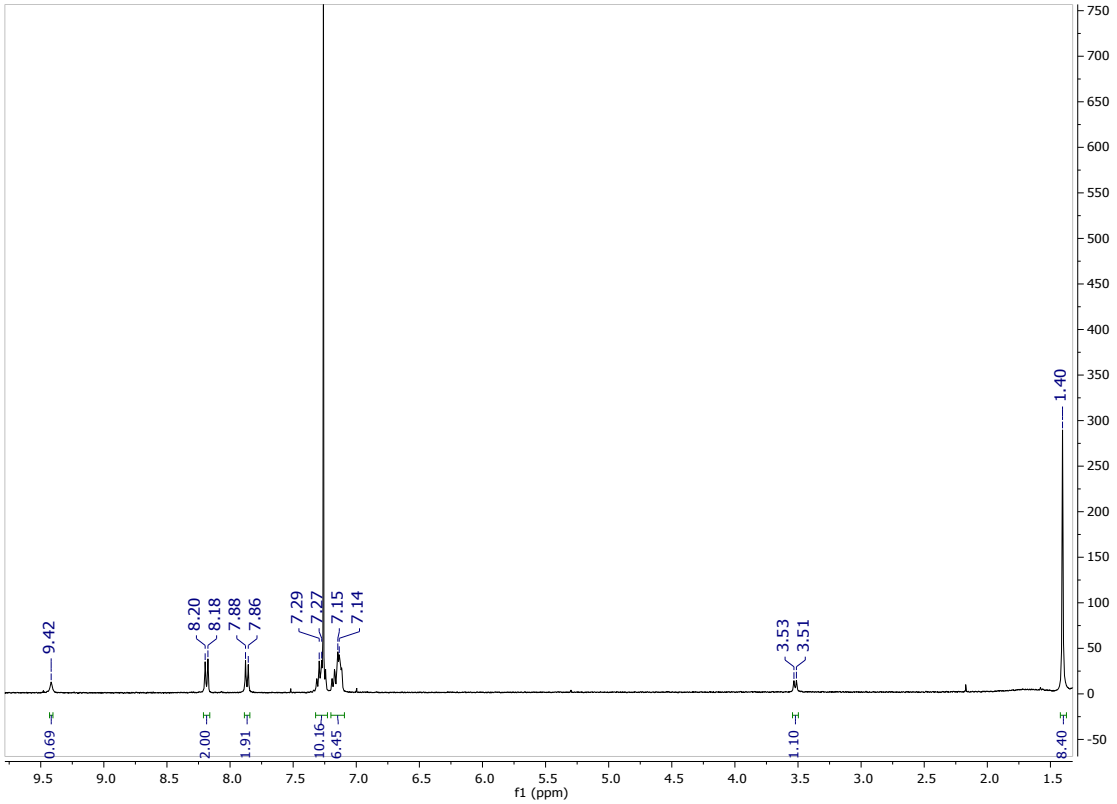


Figure S8. ^{31}P NMR spectrum of compound **[Ag(L3)$_2$]OTf (3)**

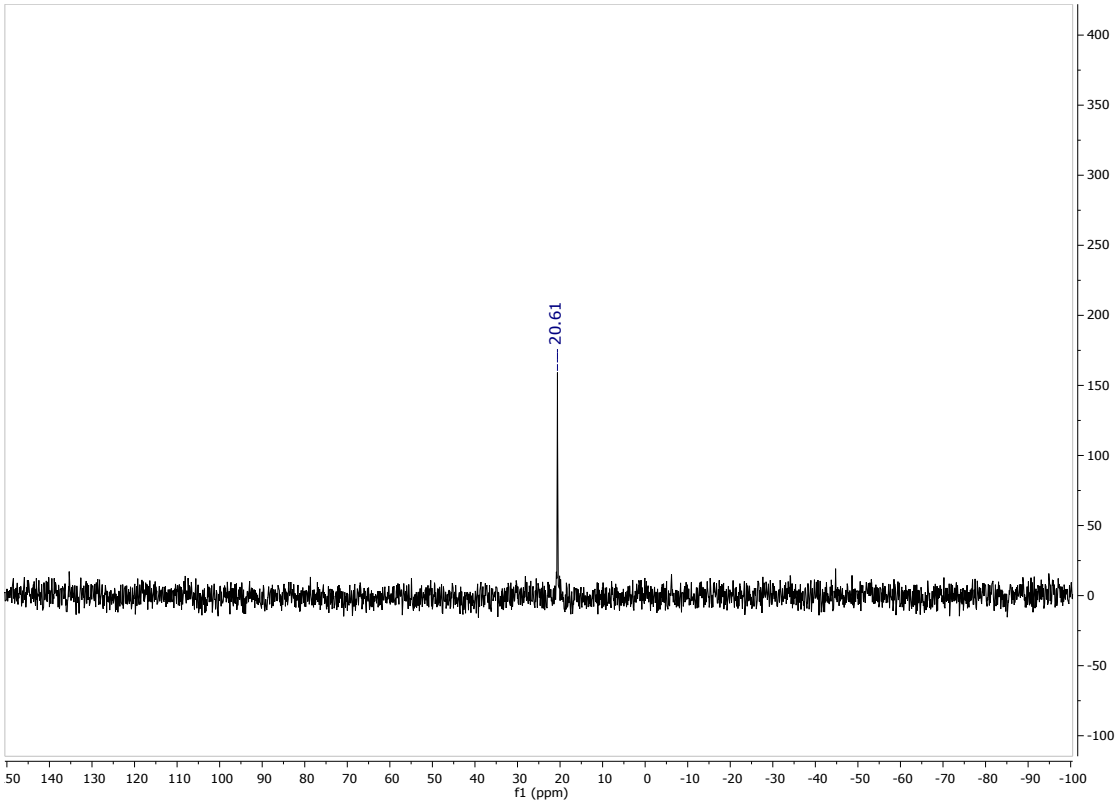
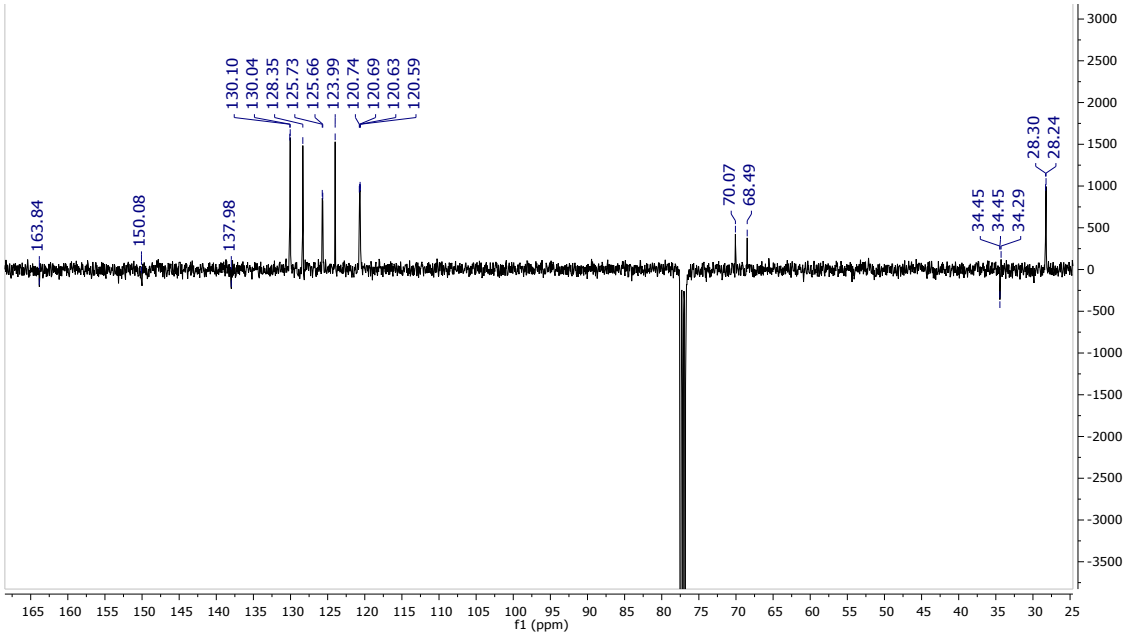


Figure S9. ^{13}C-APT spectrum of compound **[Ag(L3)$_2$]OTf (3)**



1.4. Spectra of complex $[Ag(L4)_2]OTf$ (4)

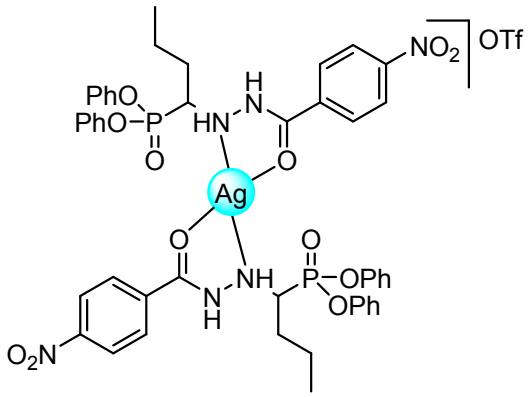


Figure S10. ^{1}H NMR spectrum of compound **$[Ag(L4)_2]OTf$ (4)**

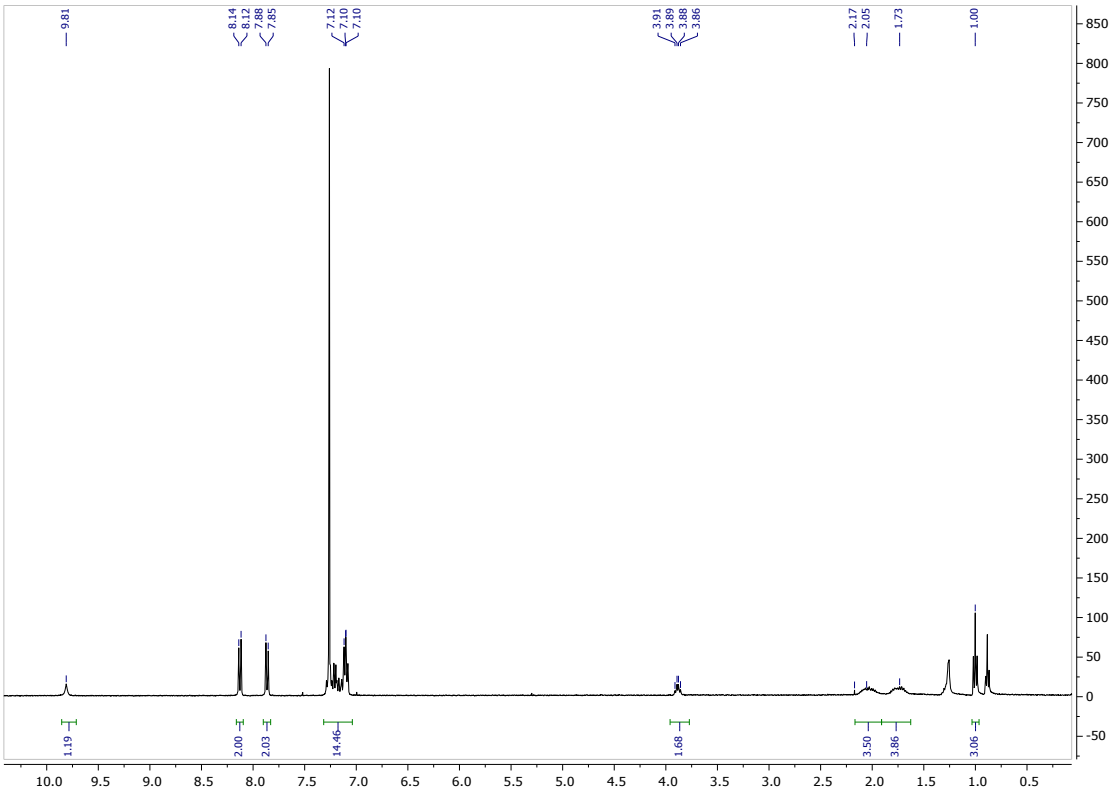


Figure S11. ^{31}P NMR spectrum of compound **[Ag(L4)$_2$]OTf (4)**

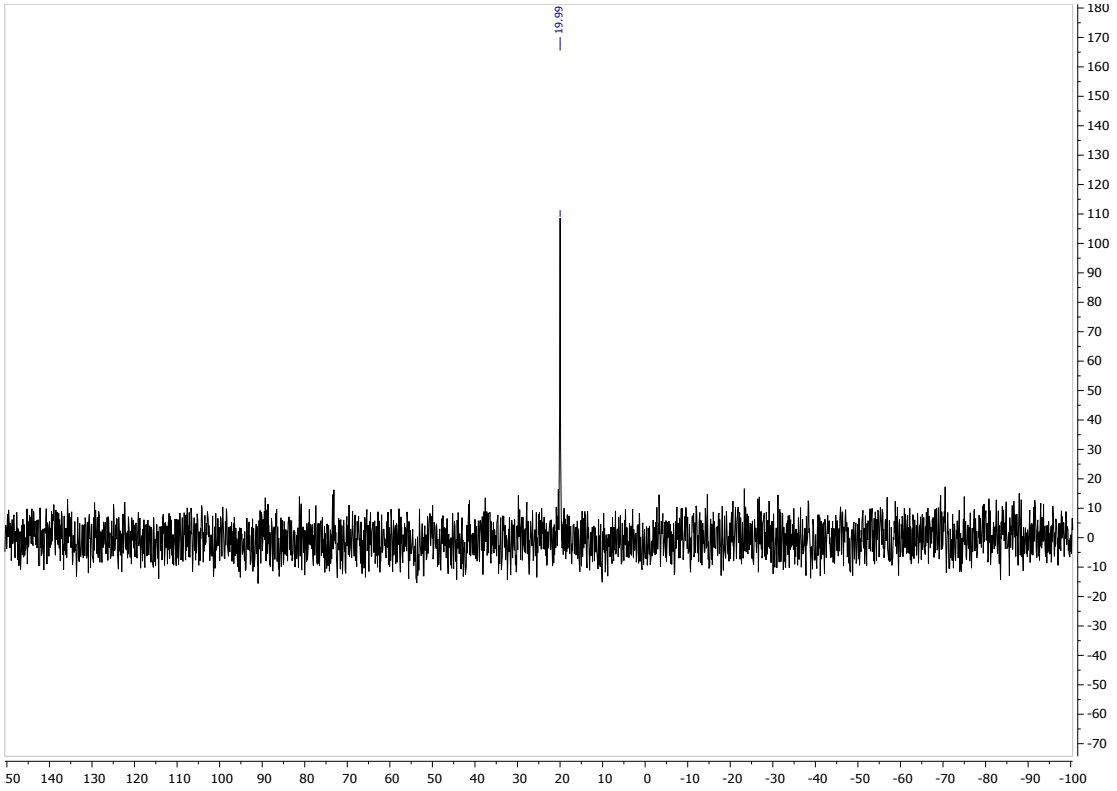
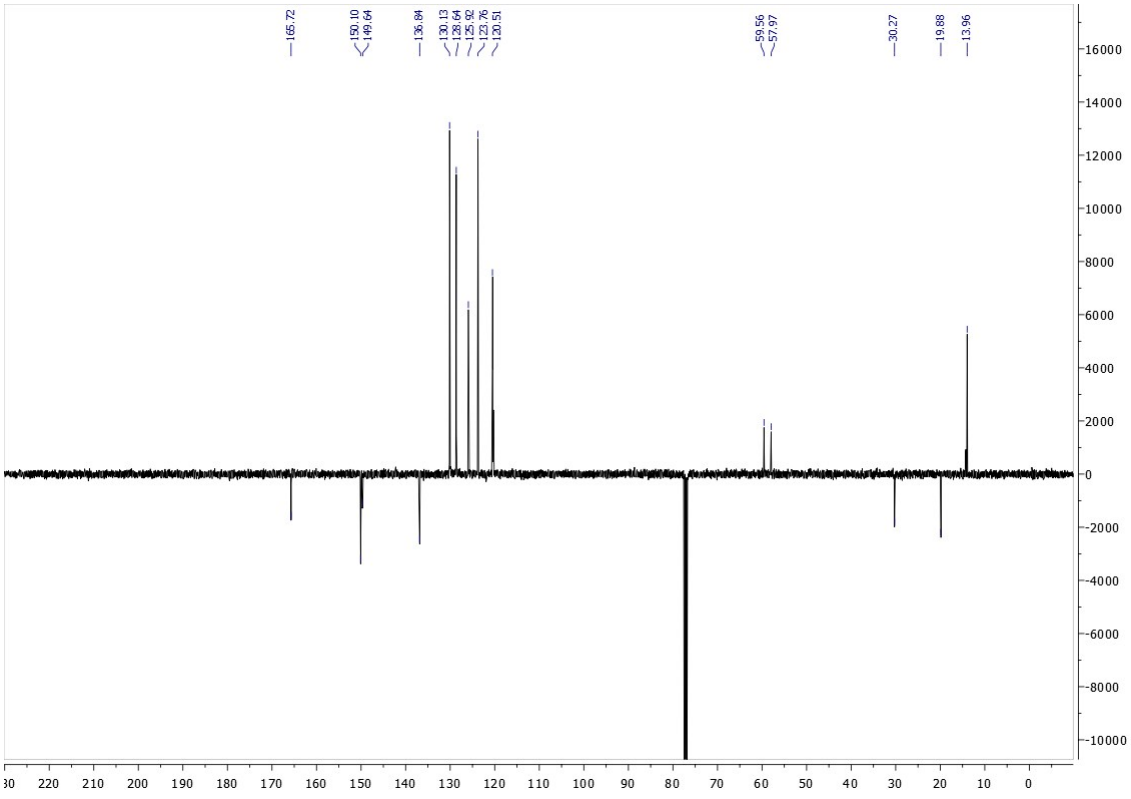


Figure S12. ^{13}C-APT spectrum of compound **[Ag(L4)$_2$]OTf (4)**



1.5. Spectra of complex [Ag(L1)(PPh$_3$)]OTf (5)

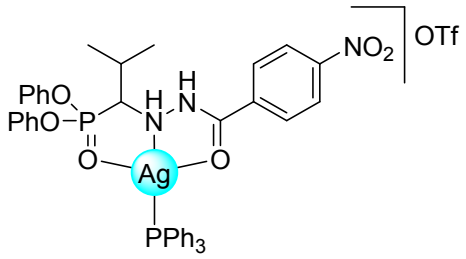


Figure S13. ^{1}H NMR spectrum of compound **[Ag(L1)(PPh$_3$)]OTf (5)**

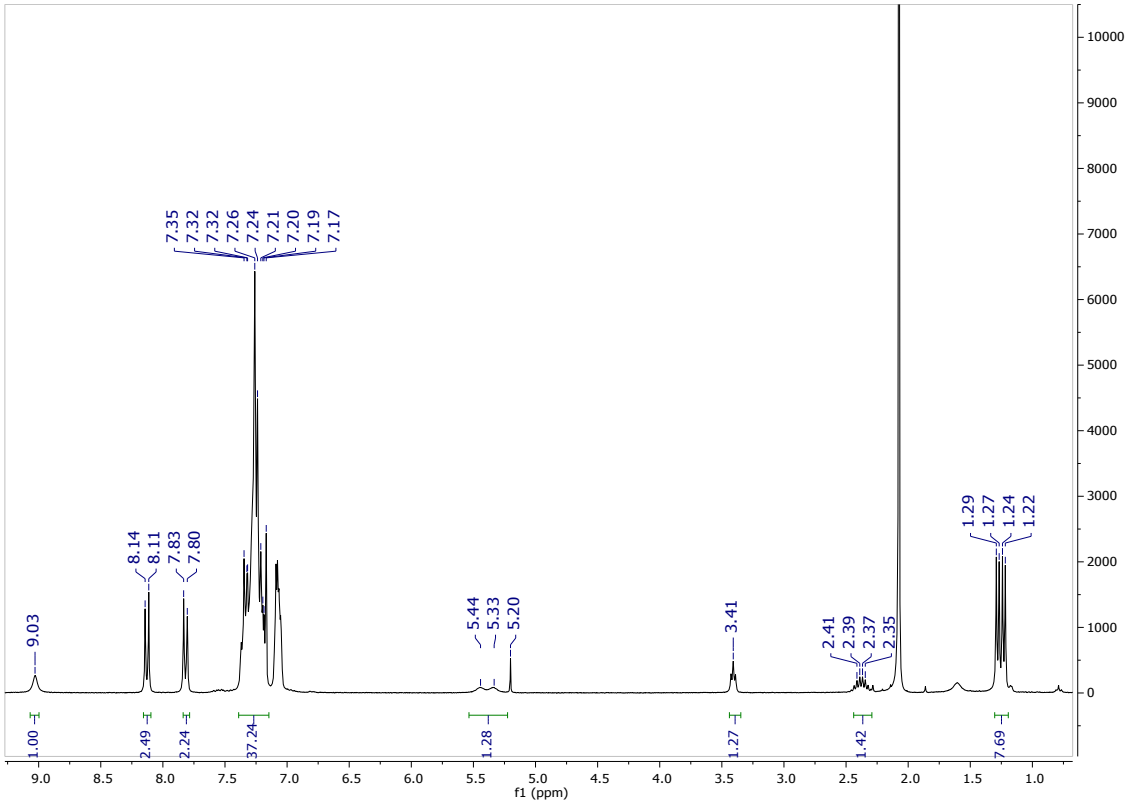


Figure S14. ^{31}P NMR spectrum of compound **[Ag(L1)(PPh$_3$)]OTf (5)**

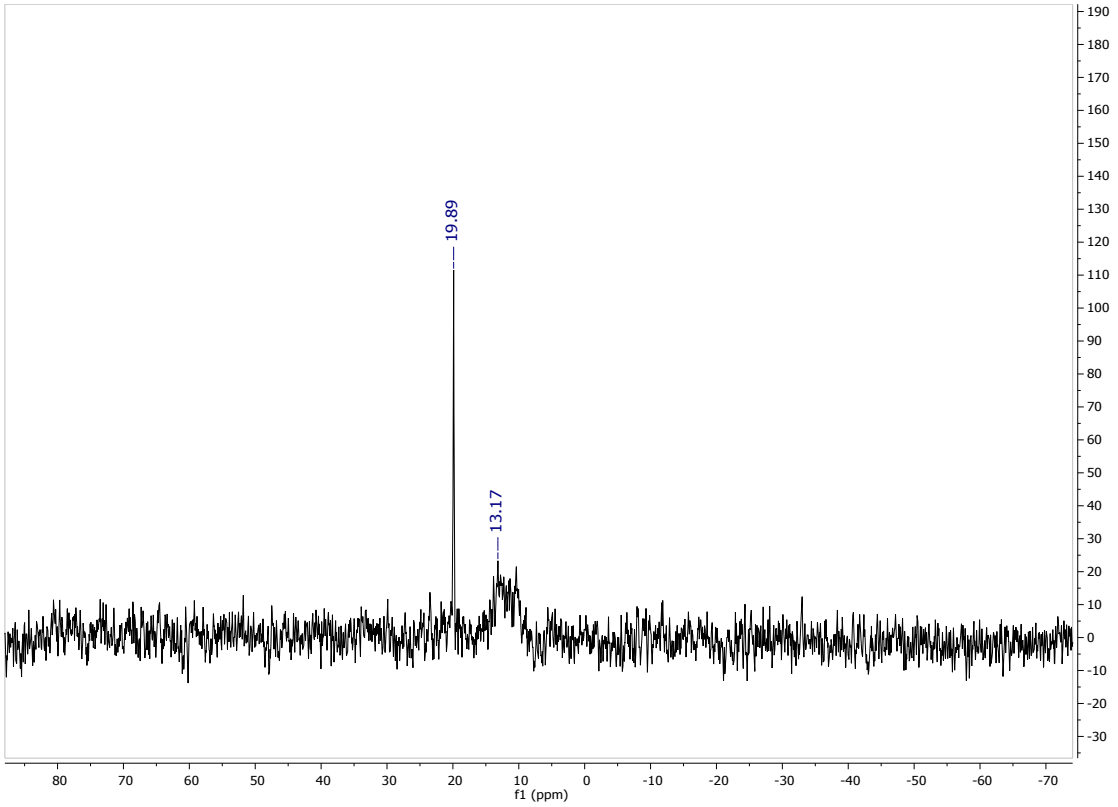
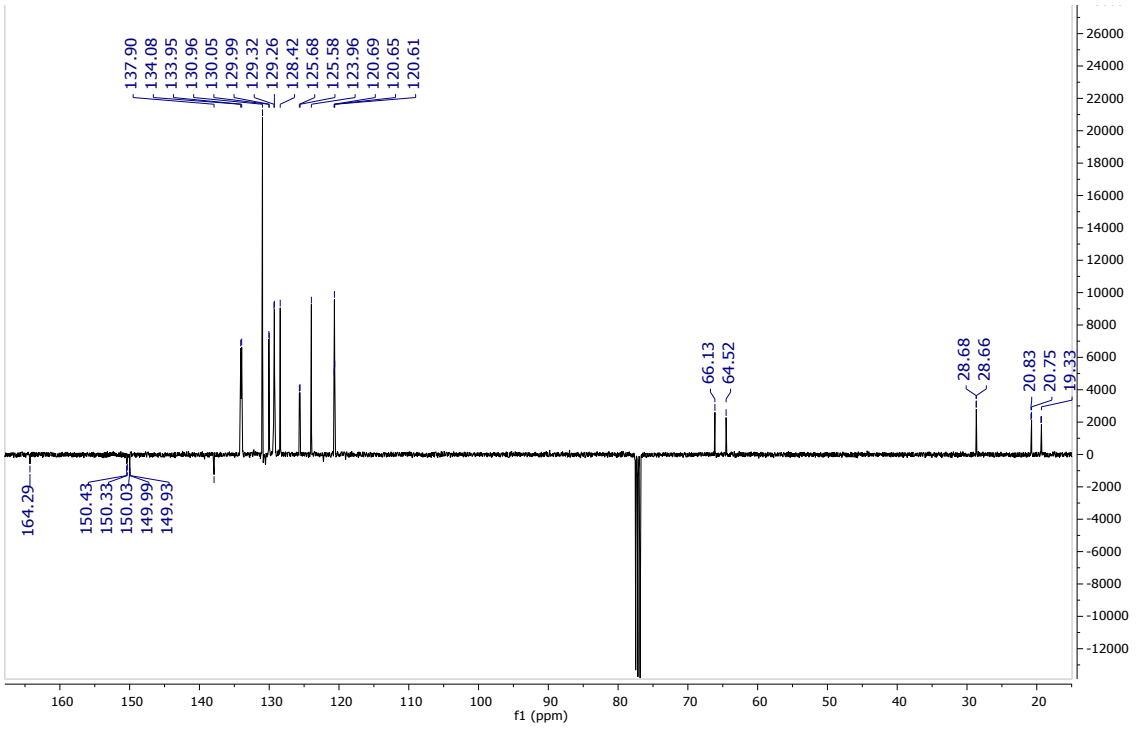


Figure S15. ^{13}C-APT spectrum of compound **[Ag(L1)(PPh$_3$)]OTf (5)**



1.6. Spectra of complex [Ag(L2)(PPh$_3$)]OTf (6)

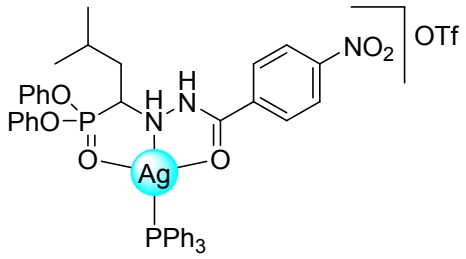


Figure S16. ^{1}H NMR spectrum of compound **[Ag(L2)(PPh$_3$)]OTf (6)**

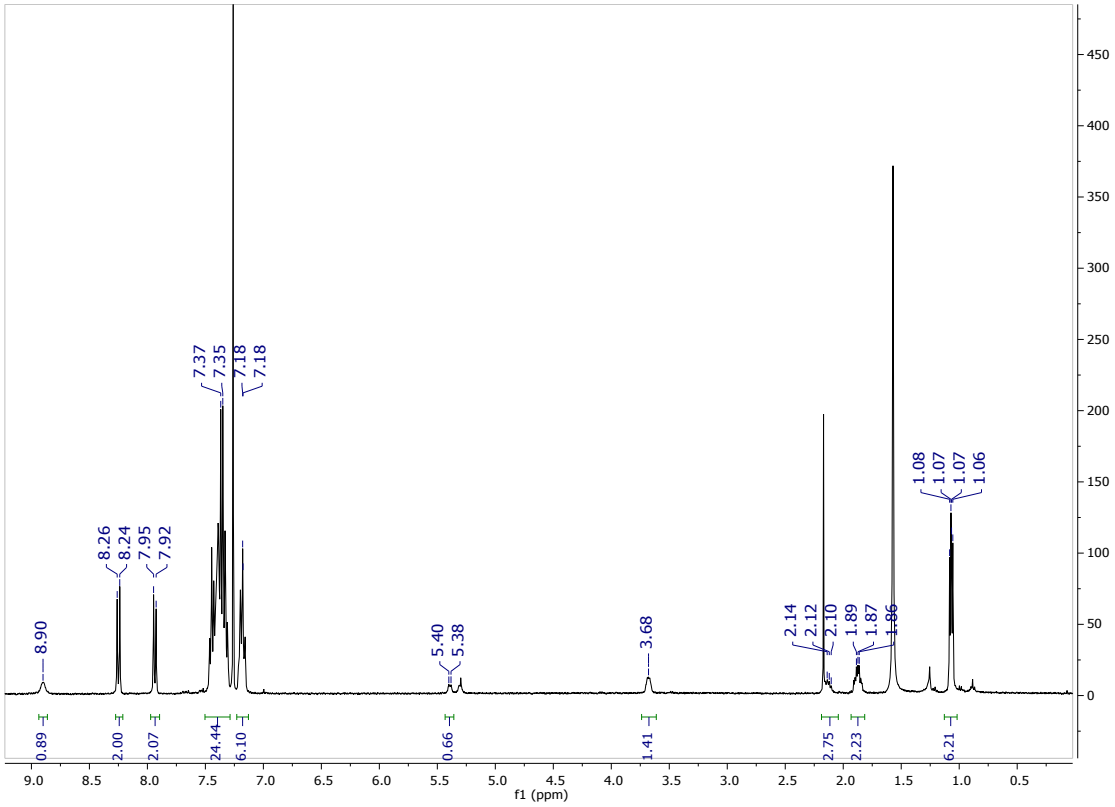


Figure S17. ^{31}P NMR spectrum of compound **[Ag(L2)(PPh$_3$)]OTf (6)**

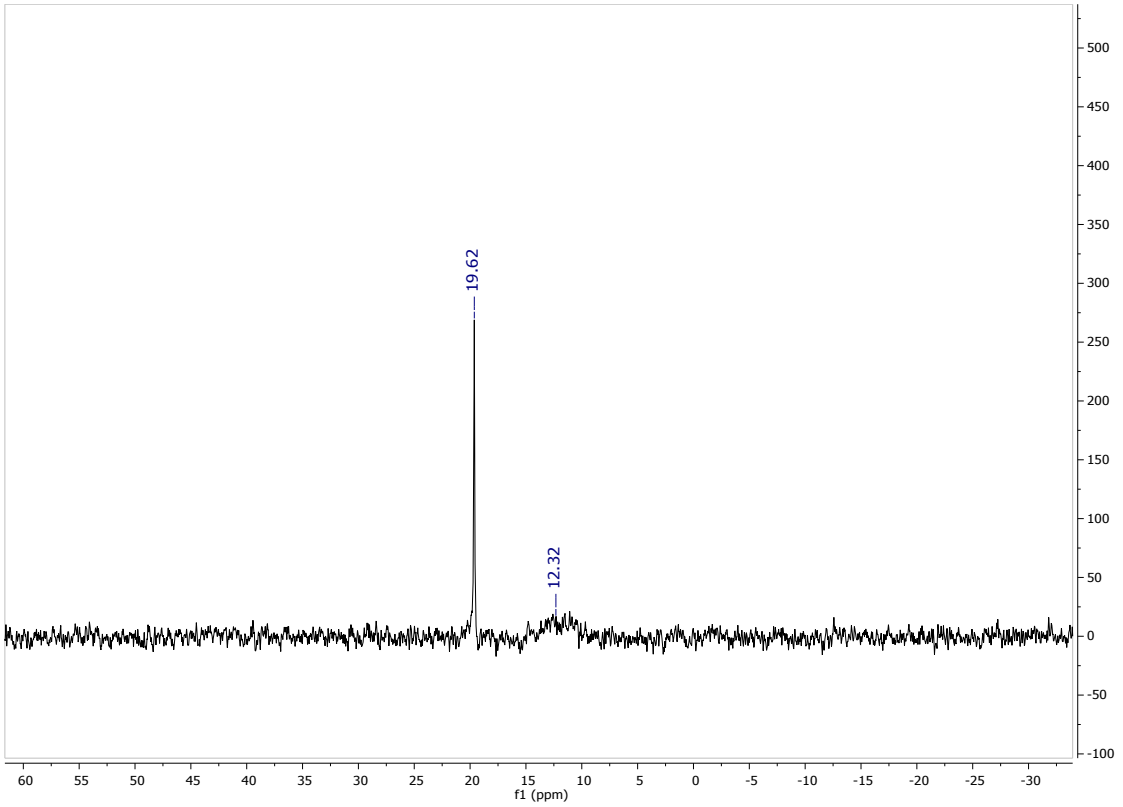
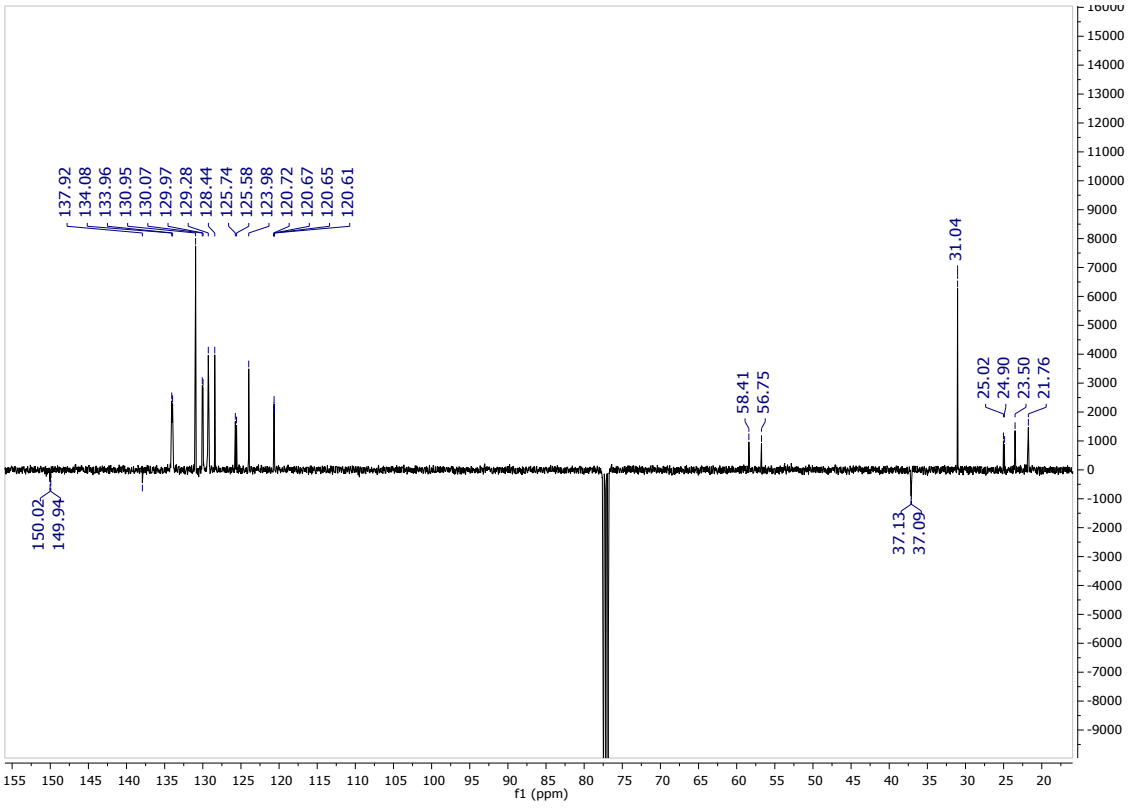


Figure S18. ^{13}C-APT spectrum of compound **[Ag(L2)(PPh$_3$)]OTf (6)**



1.7. Spectra of complex [Ag(L3)(PPh$_3$)]OTf (7)

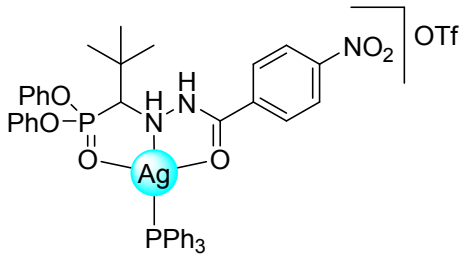


Figure S19. ^{1}H NMR spectrum of compound **[Ag(L3)(PPh$_3$)]OTf (7)**

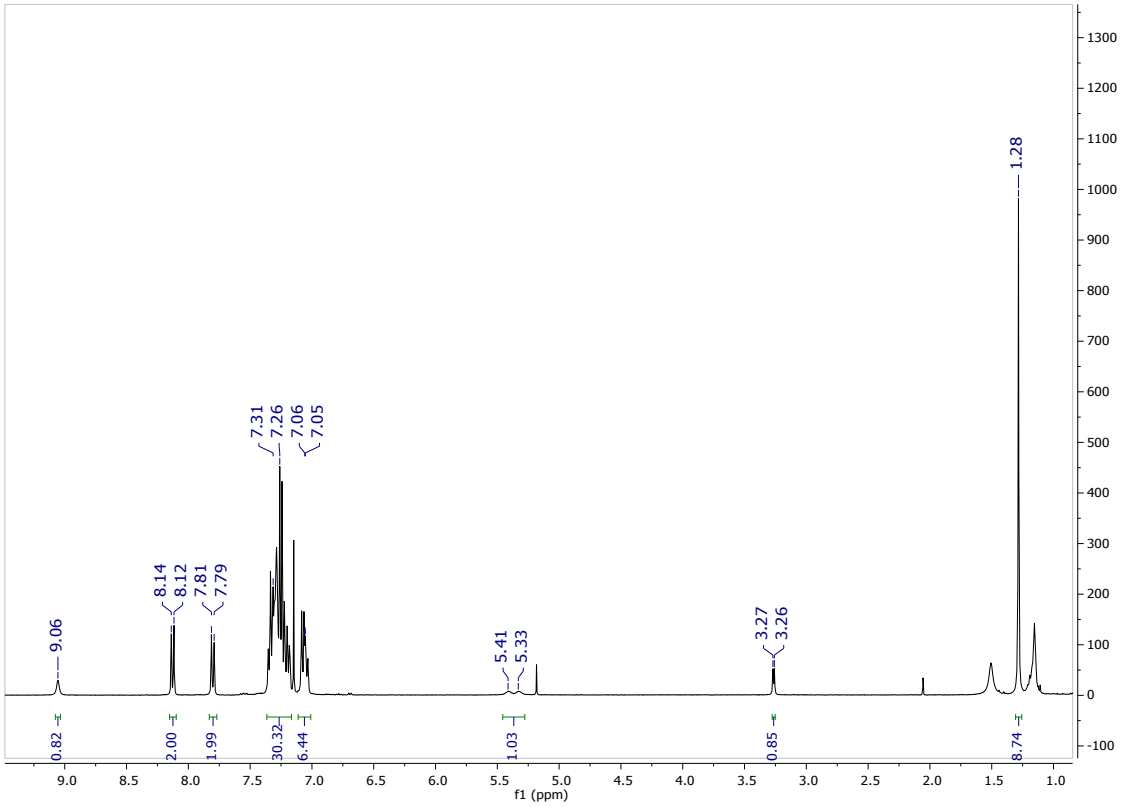


Figure S20. ^{31}P NMR spectrum of compound **[Ag(L3)(PPh$_3$)]OTf (7)**

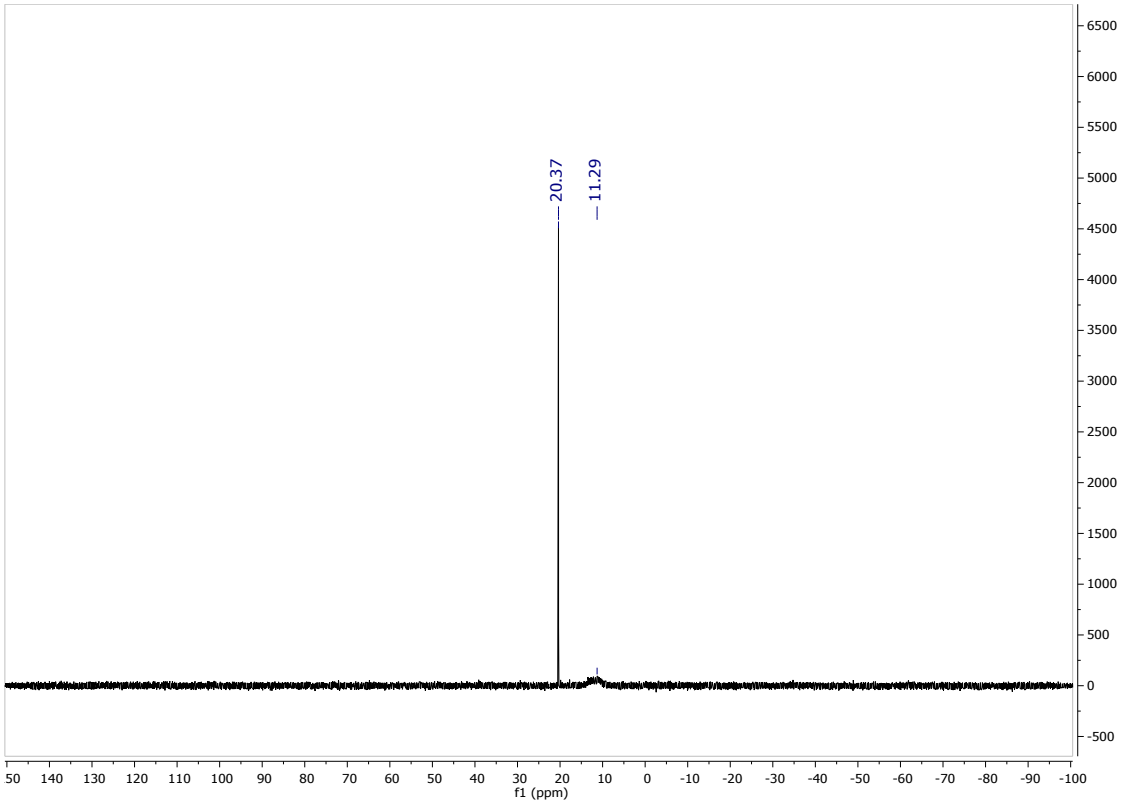
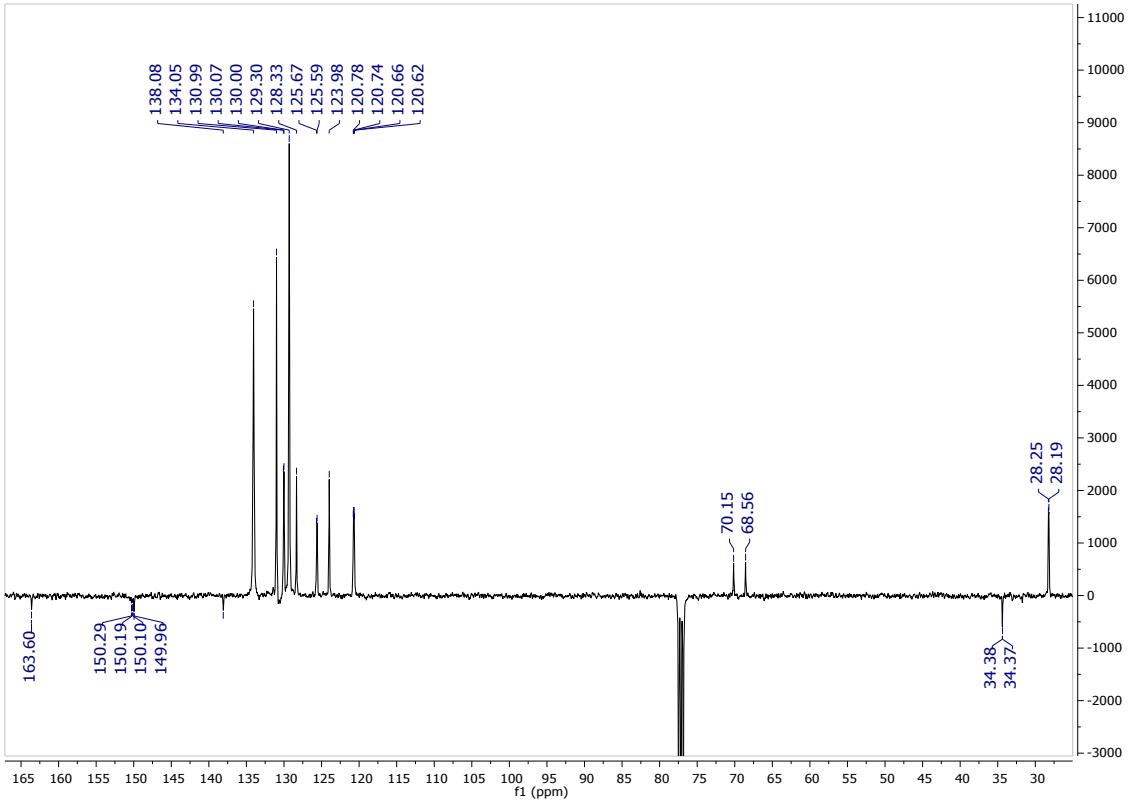


Figure S21. ^{13}C-APT spectrum of compound **[Ag(L3)(PPh$_3$)]OTf (7)**



1.8. Spectra of complex [Ag(L4)(PPh$_3$)]OTf (8)

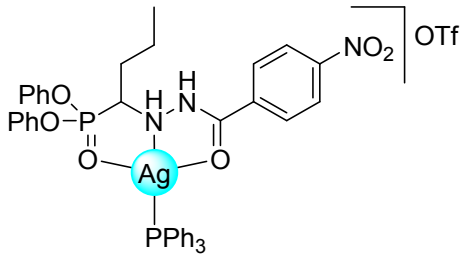


Figure S22. ^{1}H NMR spectrum of compound **[Ag(L4)(PPh$_3$)]OTf (8)**

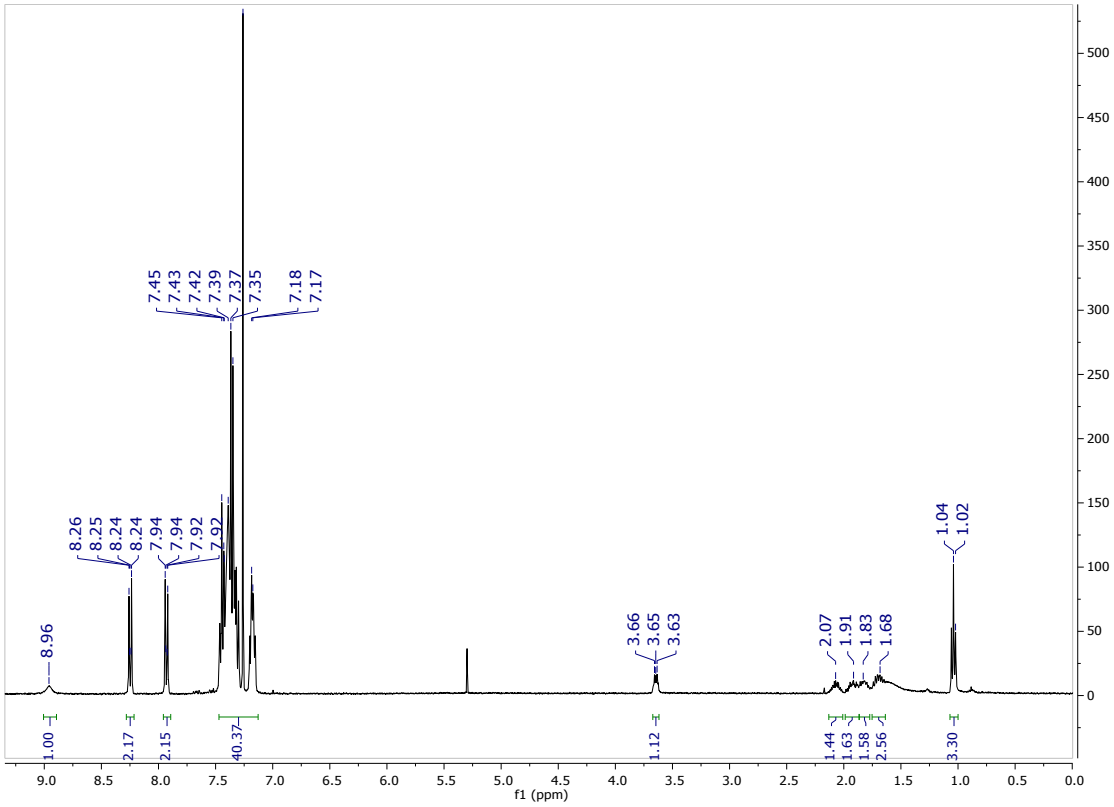


Figure S23. ^{31}P NMR spectrum of compound **[Ag(L4)(PPh$_3$)]OTf (8)**

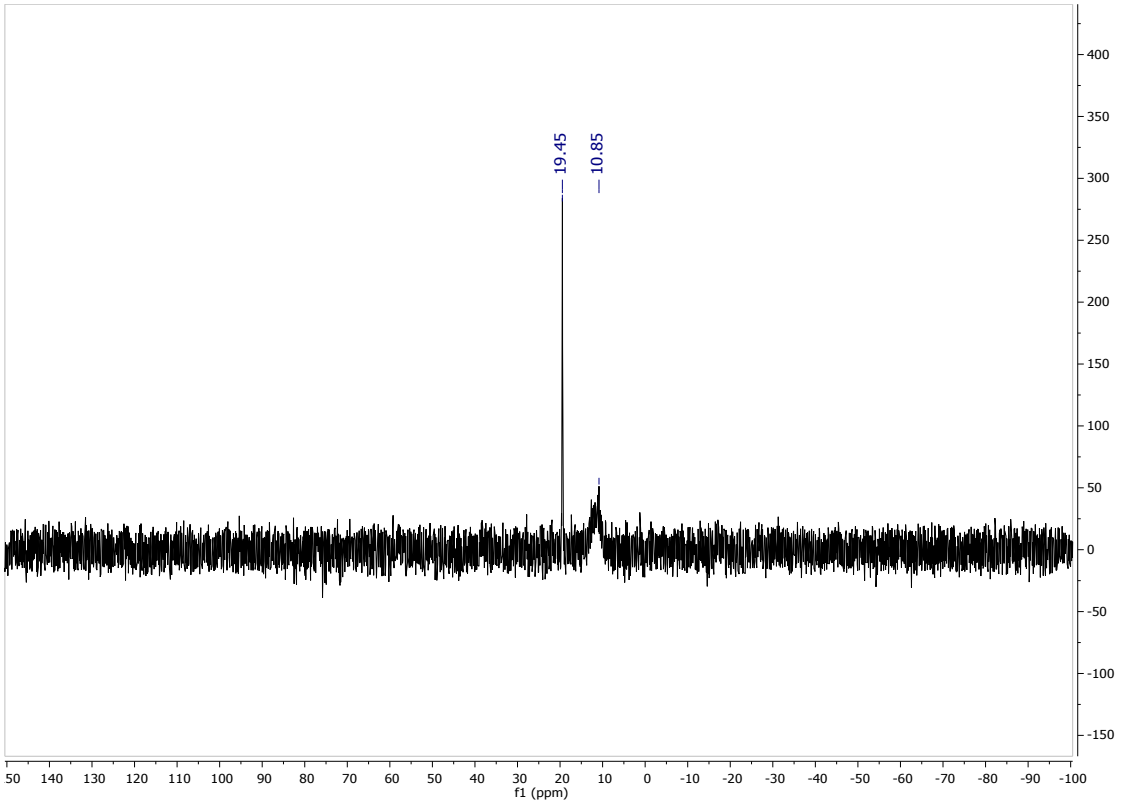
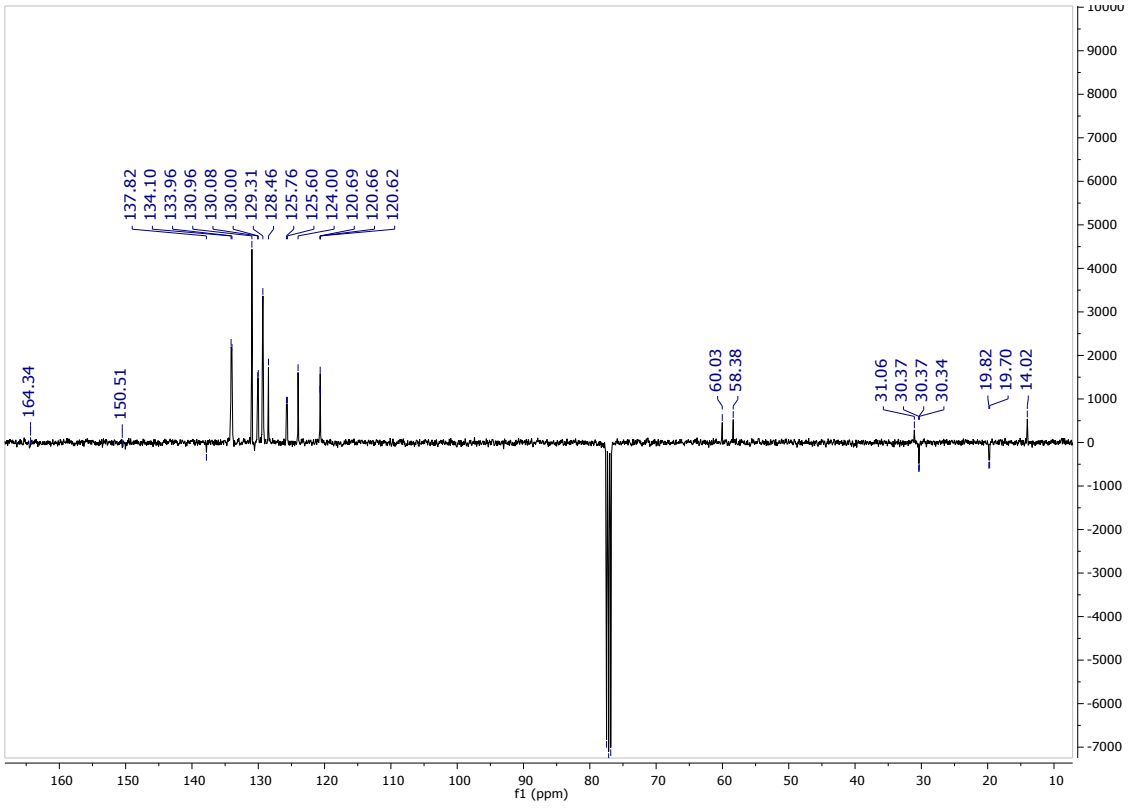


Figure S24. ^{13}C-APT spectrum of compound **[Ag(L4)(PPh$_3$)]OTf (8)**



1.9. Spectra of complex [Au(L1)(PPh$_3$)]OTf (9)

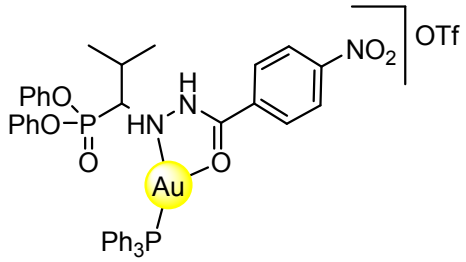


Figure S25. ^{1}H NMR spectrum of compound **[Au(L1)(PPh$_3$)]OTf (9)**

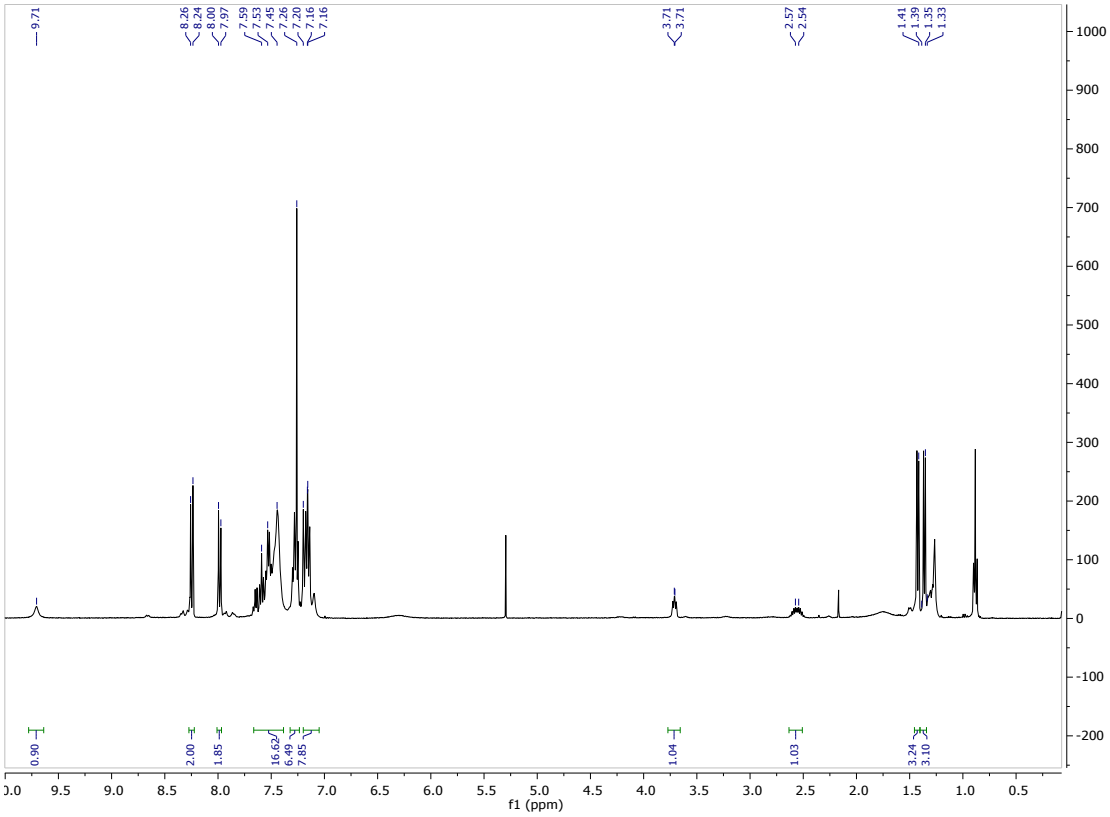


Figure S26. ^{31}P NMR spectrum of compound **[Au(L1)(PPh$_3$)]OTf (9)**

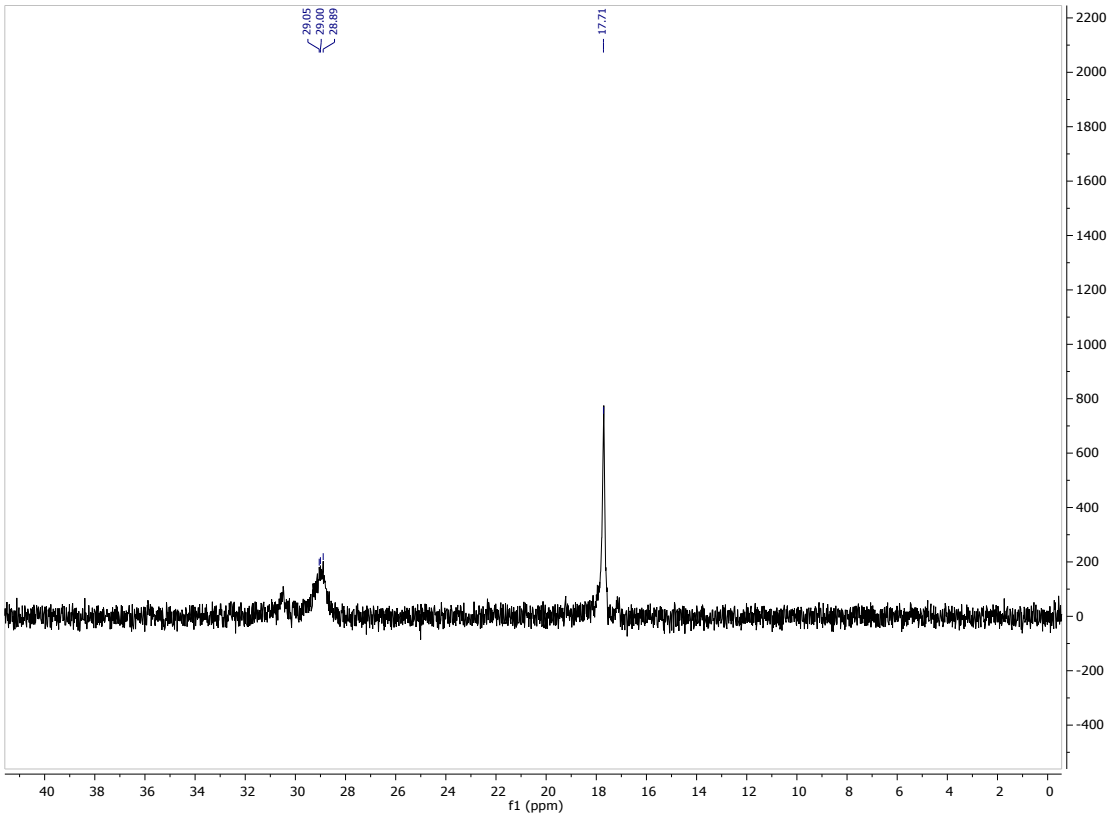
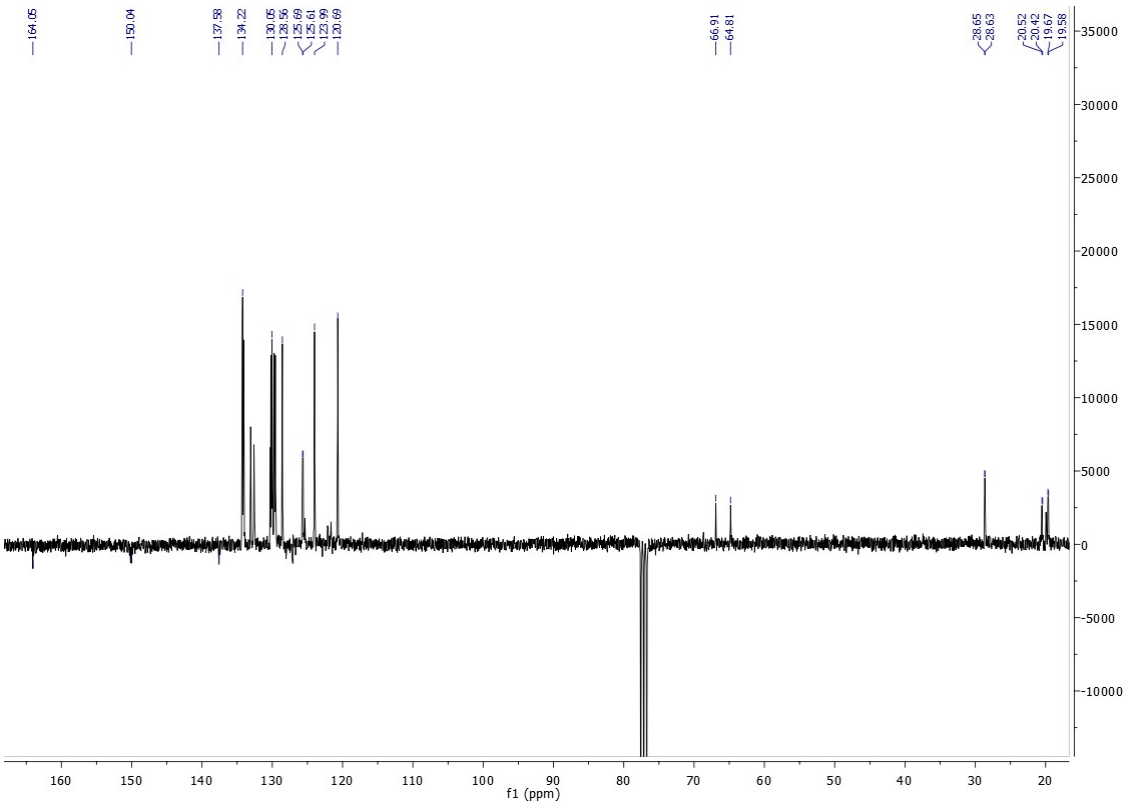


Figure S27. ^{13}C-APT spectrum of compound **[Au(L1)(PPh$_3$)]OTf (9)**



1.10. Spectra of complex [Au(L2)(PPh_3)]OTf (10)

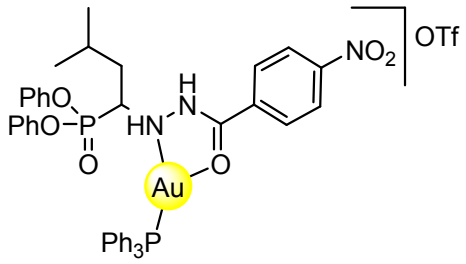


Figure S28. ^{1}H NMR spectrum of compound **[Au(L2)(PPh_3)]OTf (10)**

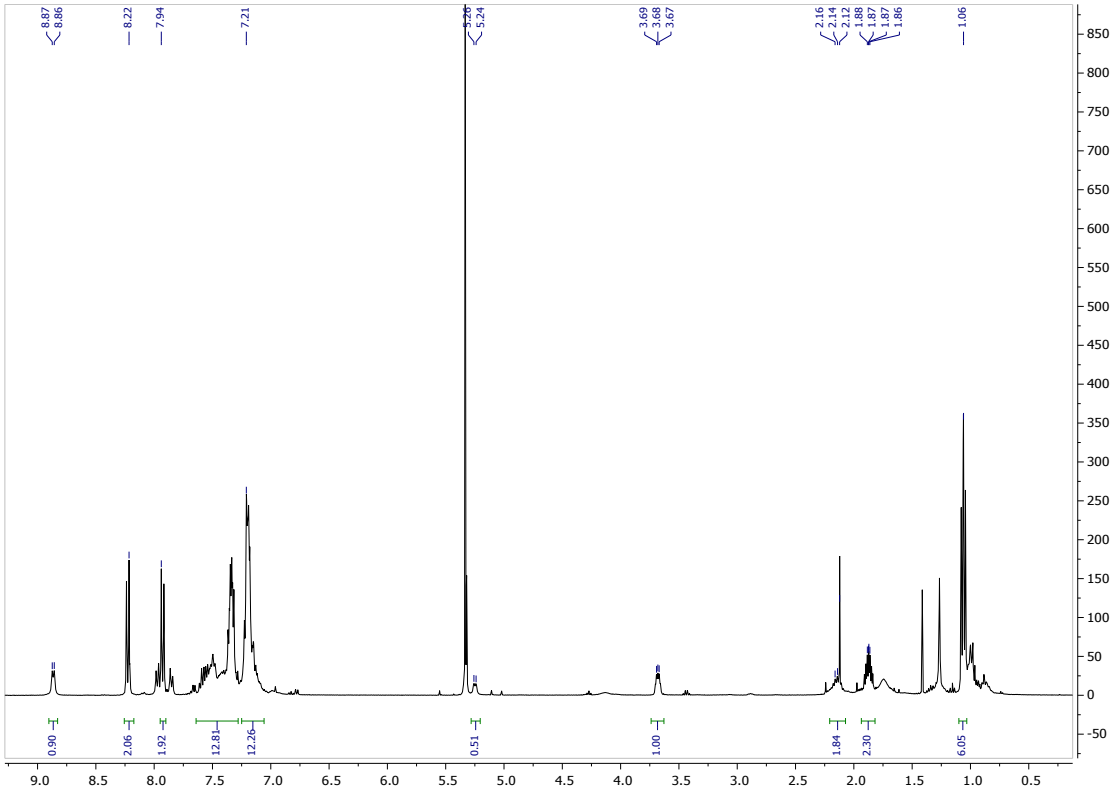


Figure S29. ^{31}P NMR spectrum of compound **[Au(L2)(PPh$_3$)]OTf (10)**

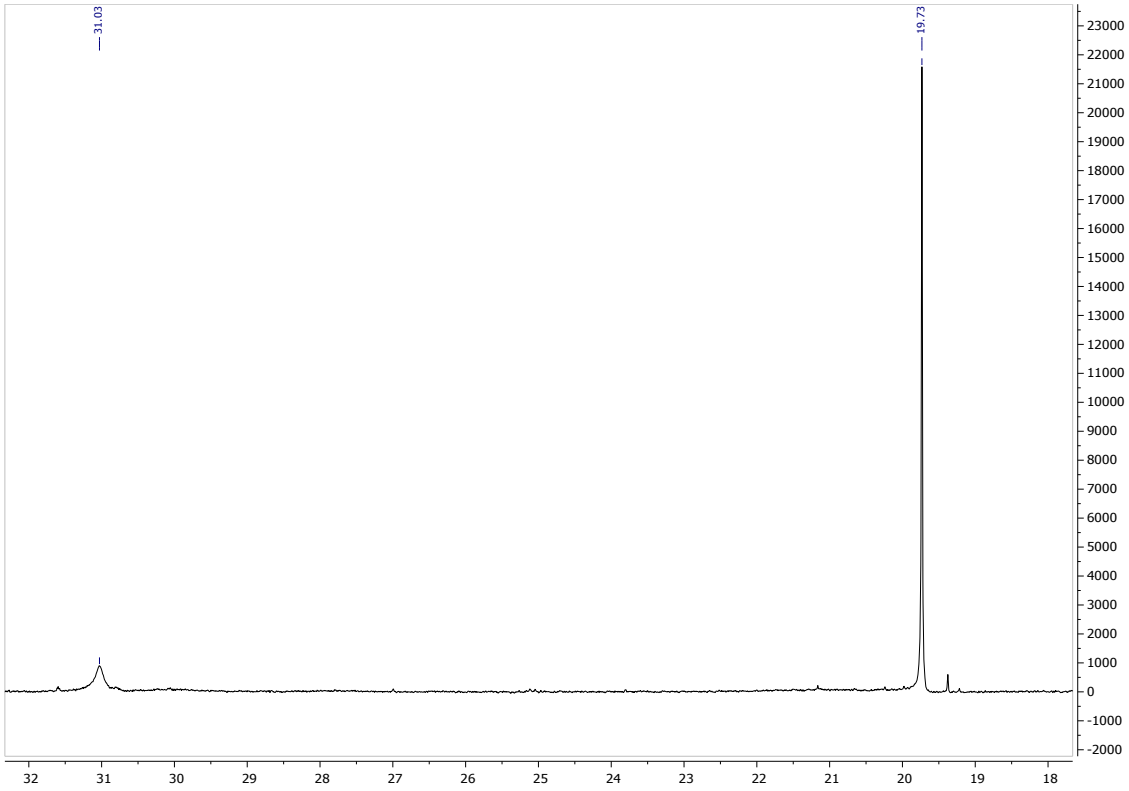
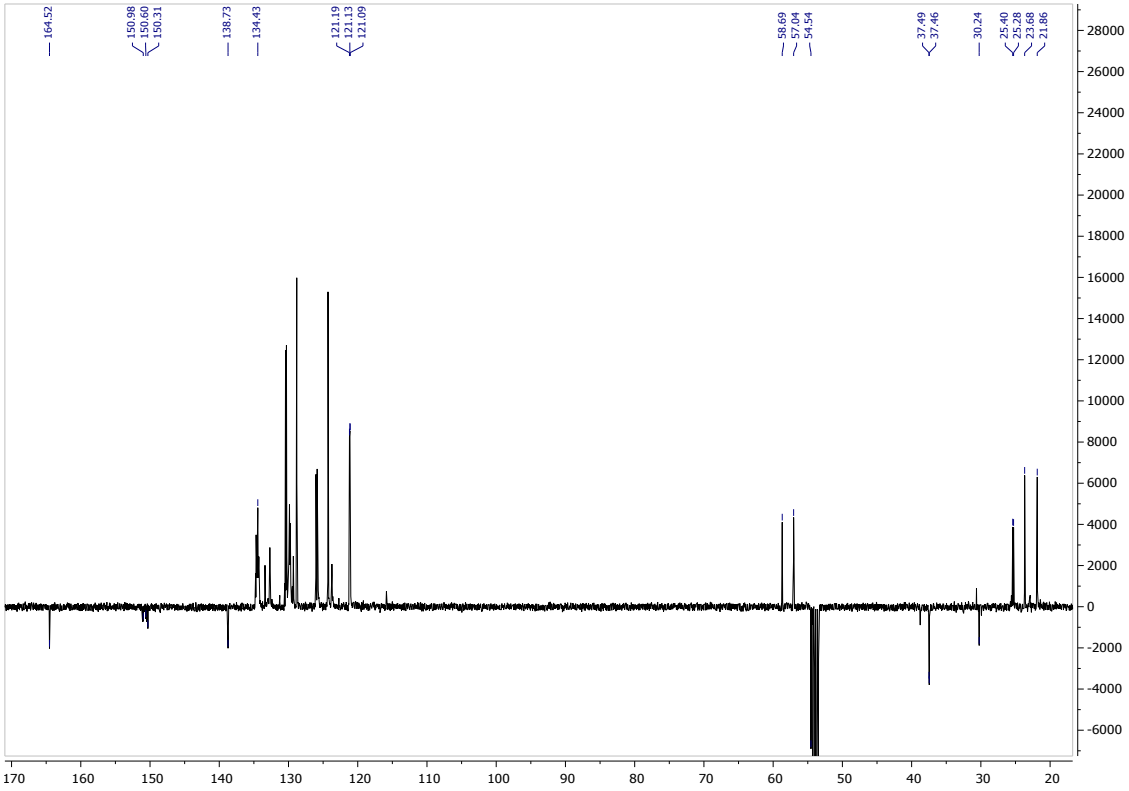


Figure S30. ^{13}C-APT spectrum of compound **[Au(L2)(PPh$_3$)]OTf (10)**



1.11. Spectra of complex [Au(L4)(PPh_3)]OTf (11)

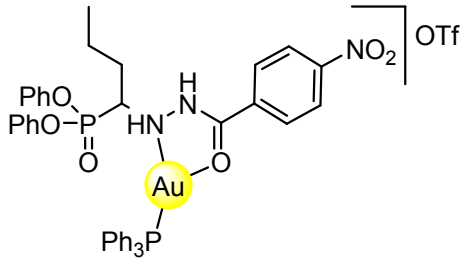


Figure S31. ^{1}H NMR spectrum of compound **[Au(L4)(PPh_3)]OTf (11)**

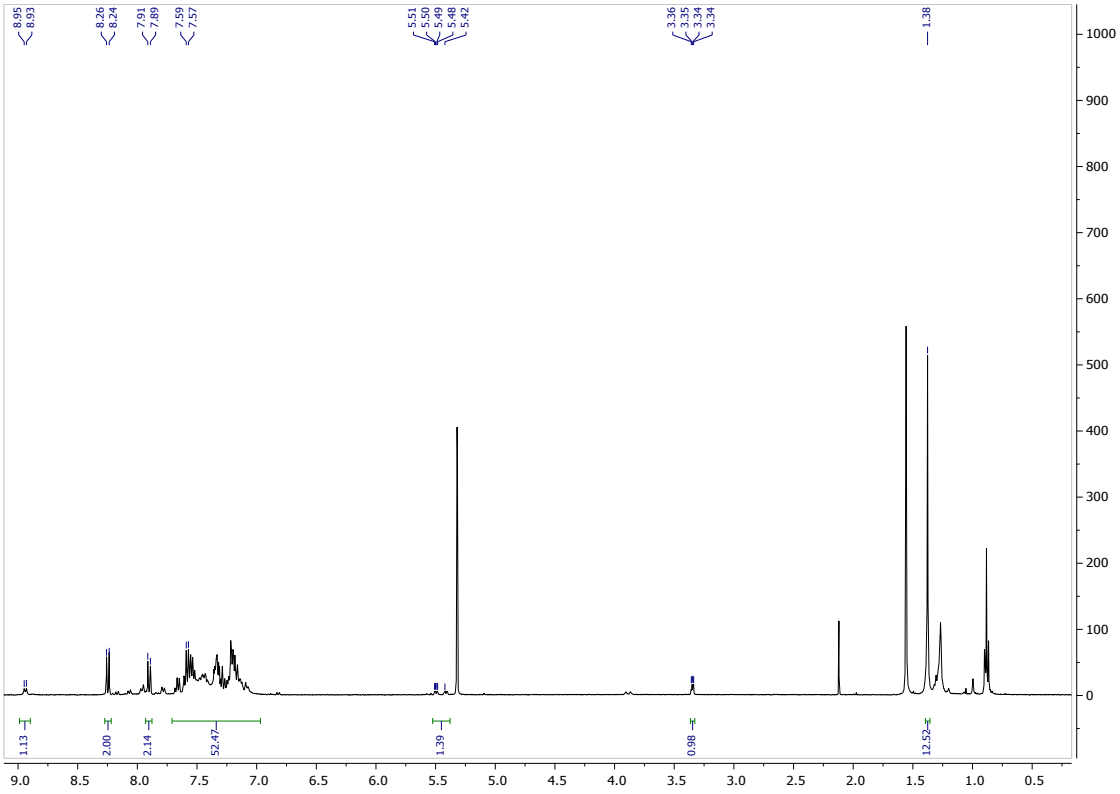


Figure S32. ^{31}P NMR spectrum of compound **[Au(L4)(PPh$_3$)]OTf (11)**

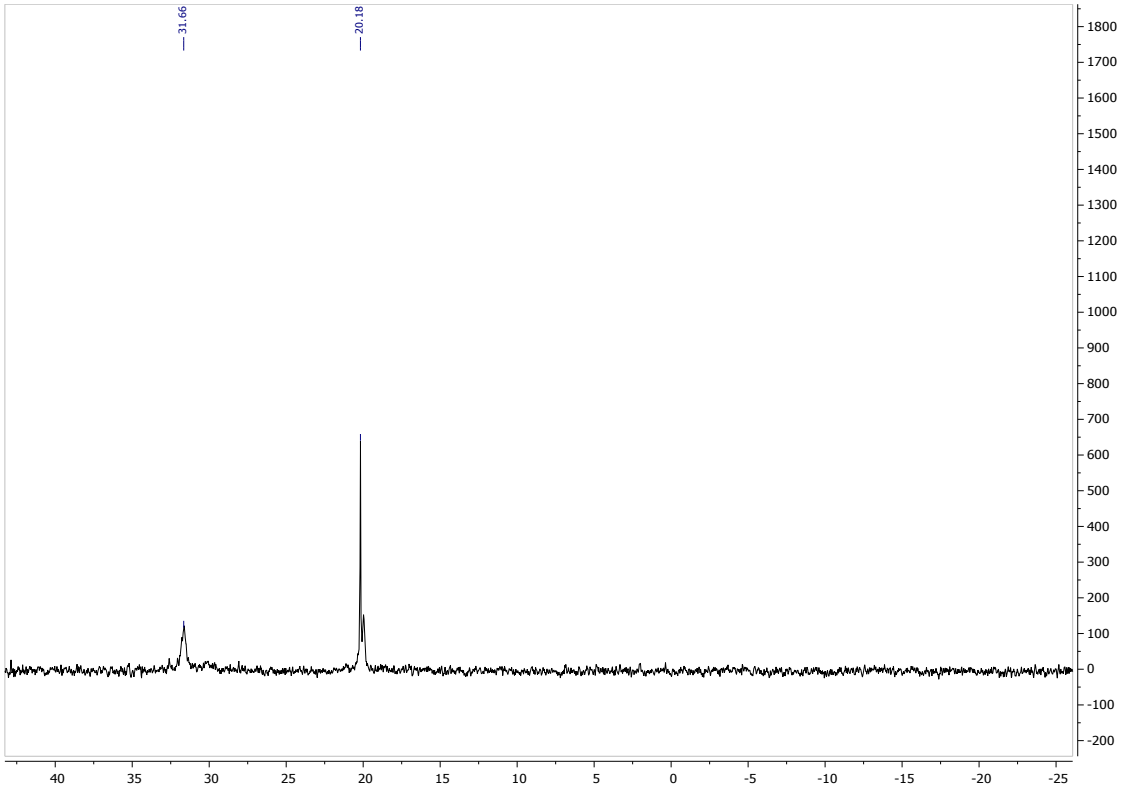
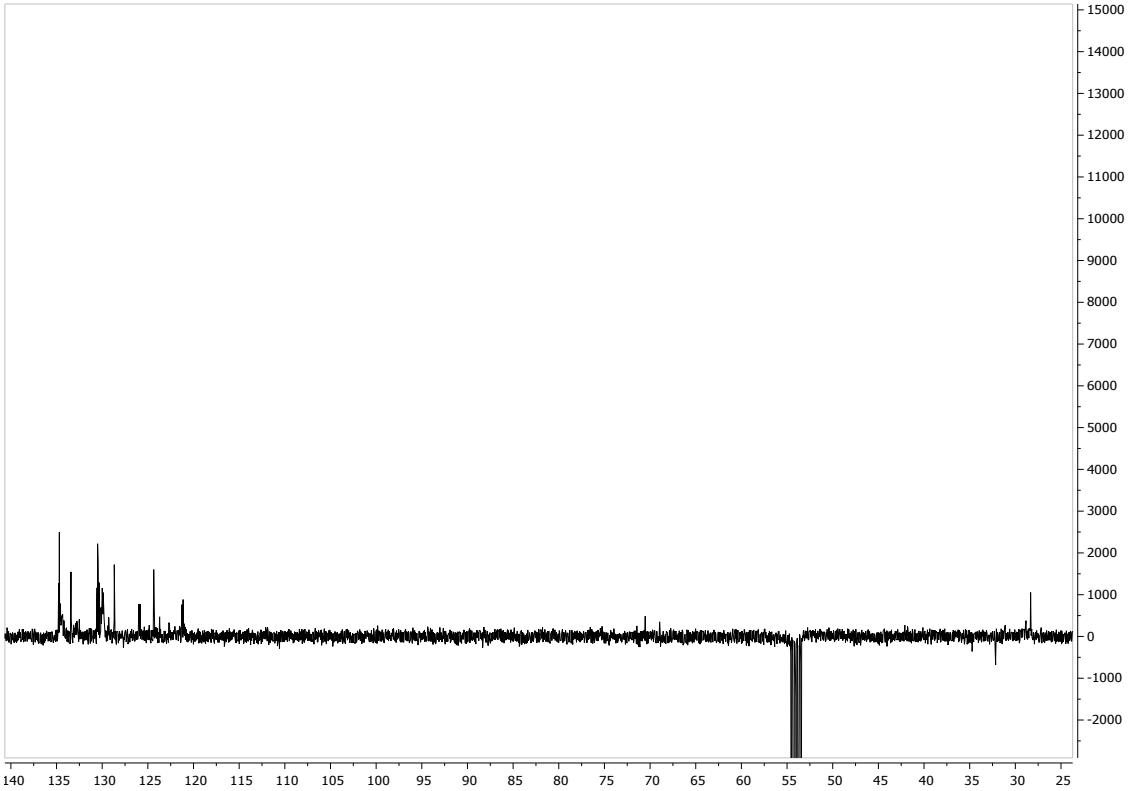


Figure S33. ^{13}C-APT spectrum of compound **[Au(L4)(PPh$_3$)]OTf (11)**



1.12. Spectra of complex [Au(L2)$_2$]OTf (12)

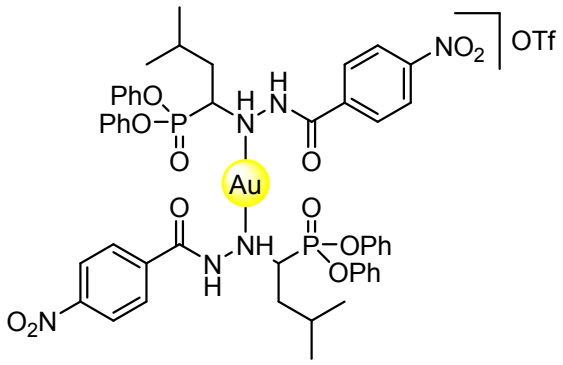


Figure S34. ^{1}H NMR spectrum of compound **[Au(L2)$_2$]OTf (12)**

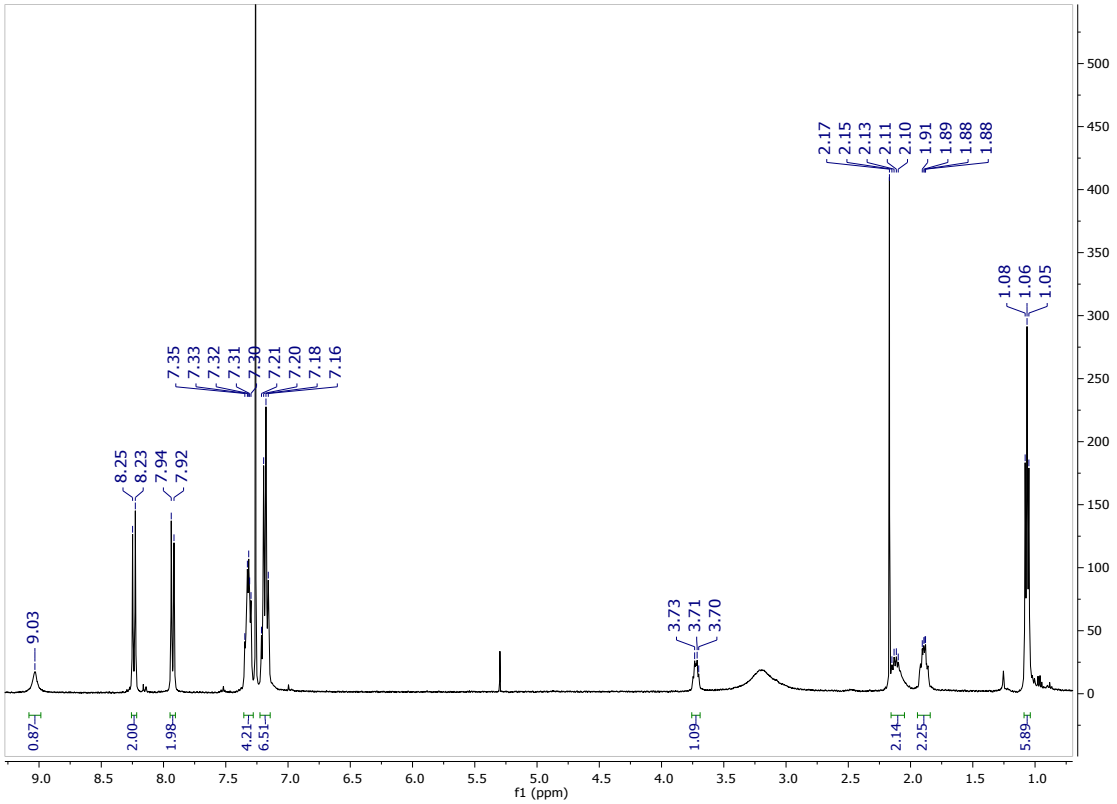


Figure S35. ^{31}P NMR spectrum of compound **[Au(L2)$_2$]OTf (12)**

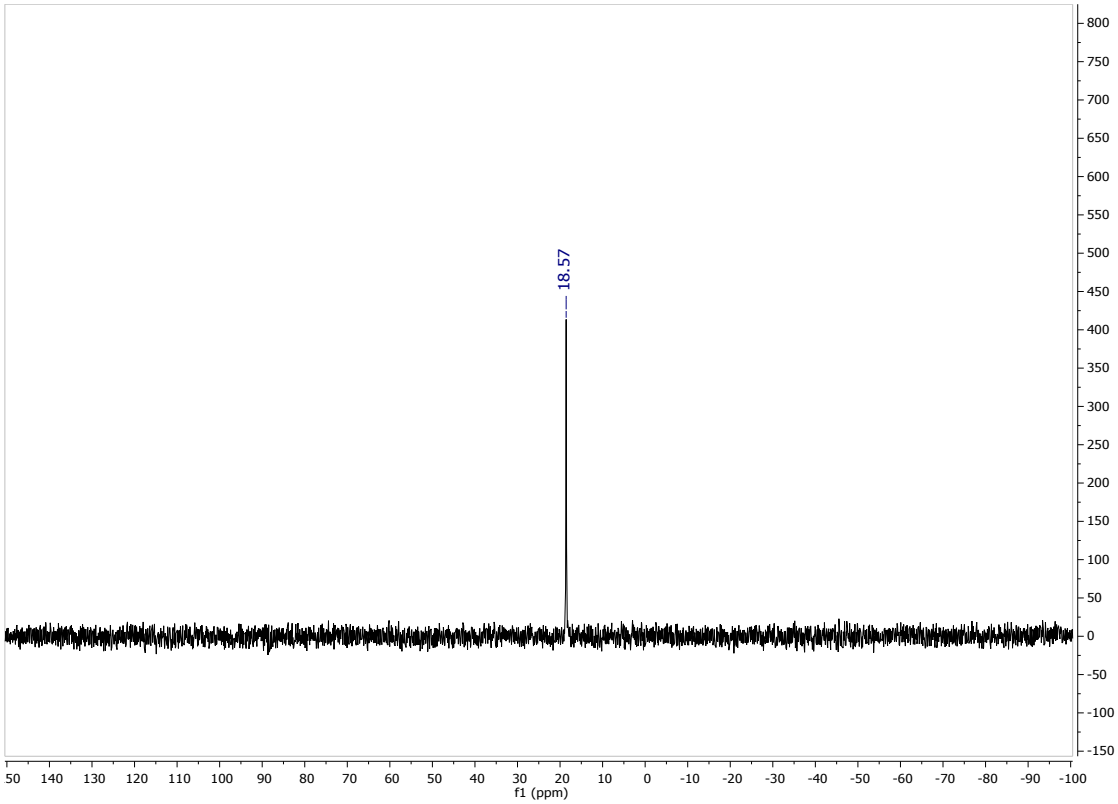
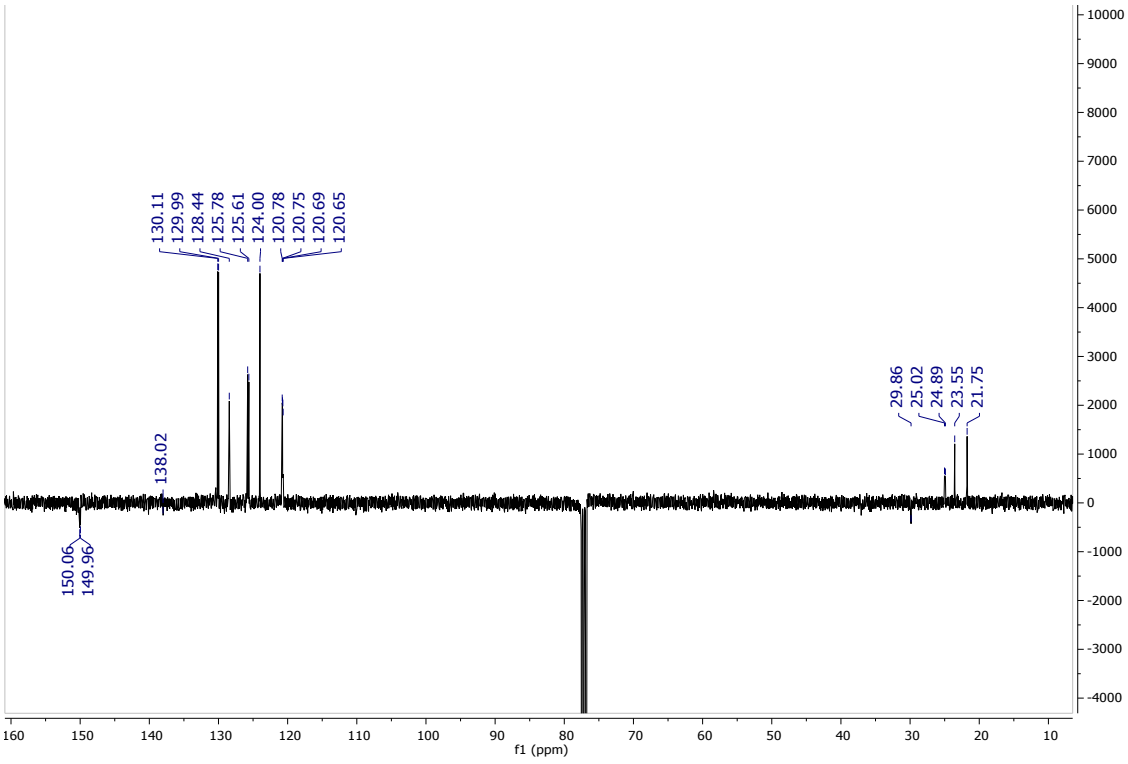


Figure S36. ^{13}C-APT spectrum of compound **[Au(L2)$_2$]OTf (12)**



1.13. Spectra of complex $[Cu(L1)(PPh_3)]NO_3$ (13)

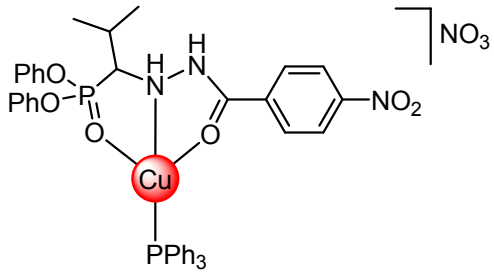


Figure S37. ^{1}H NMR spectrum of compound **$[Cu(L1)(PPh_3)]NO_3$ (13)**

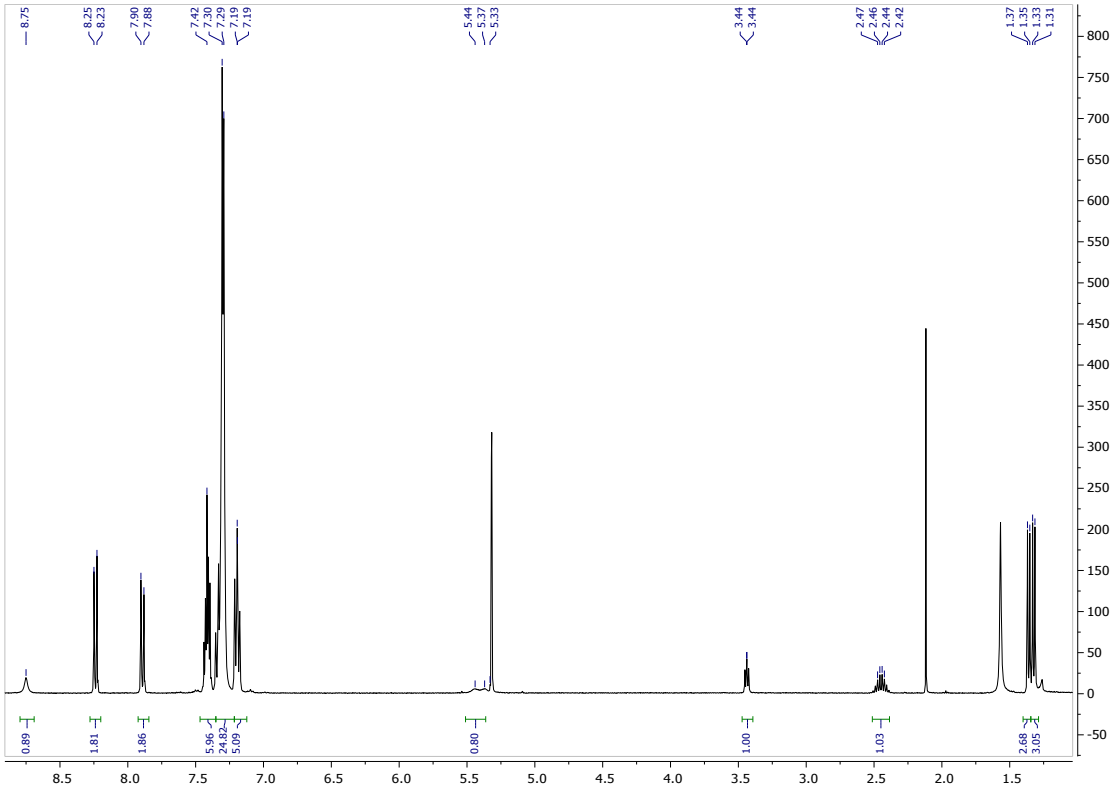


Figure S38. ^{31}P NMR spectrum of compound **[Cu(L1)(PPh$_3$)]NO$_3$ (13)**

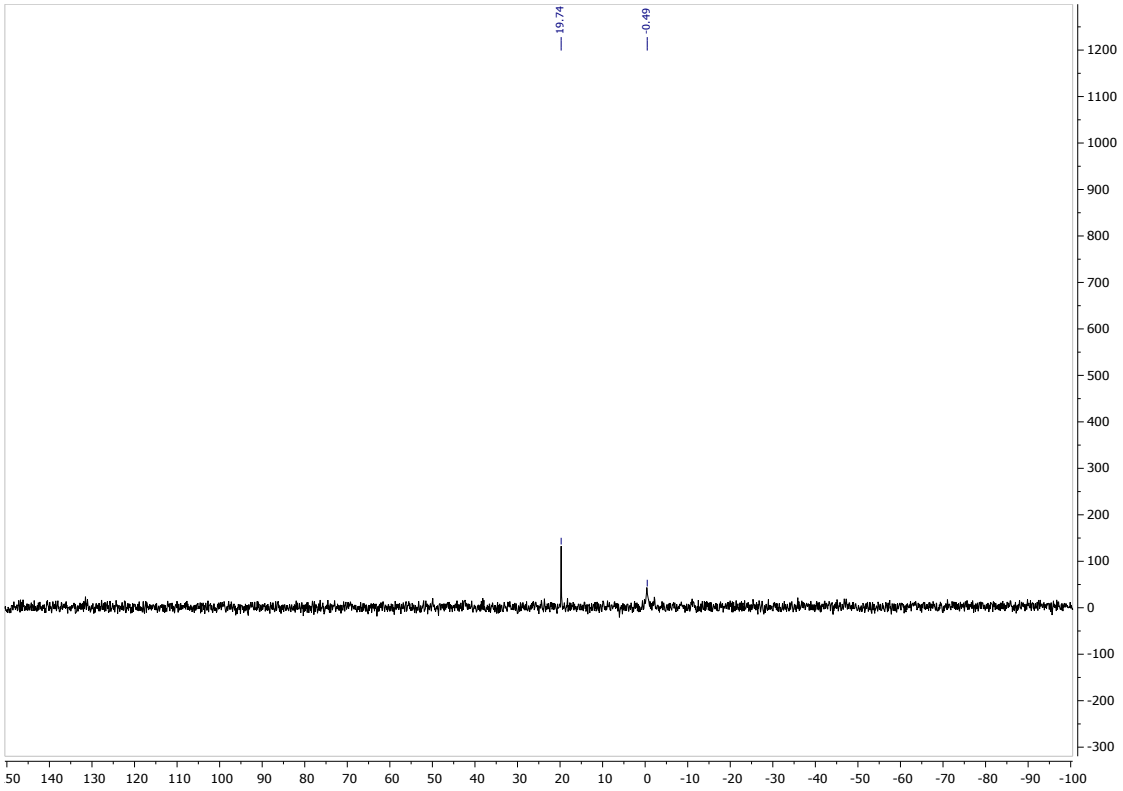


Figure S39. ^{13}C-APT spectrum of compound **[Cu(L1)(PPh$_3$)]NO$_3$ (13)**

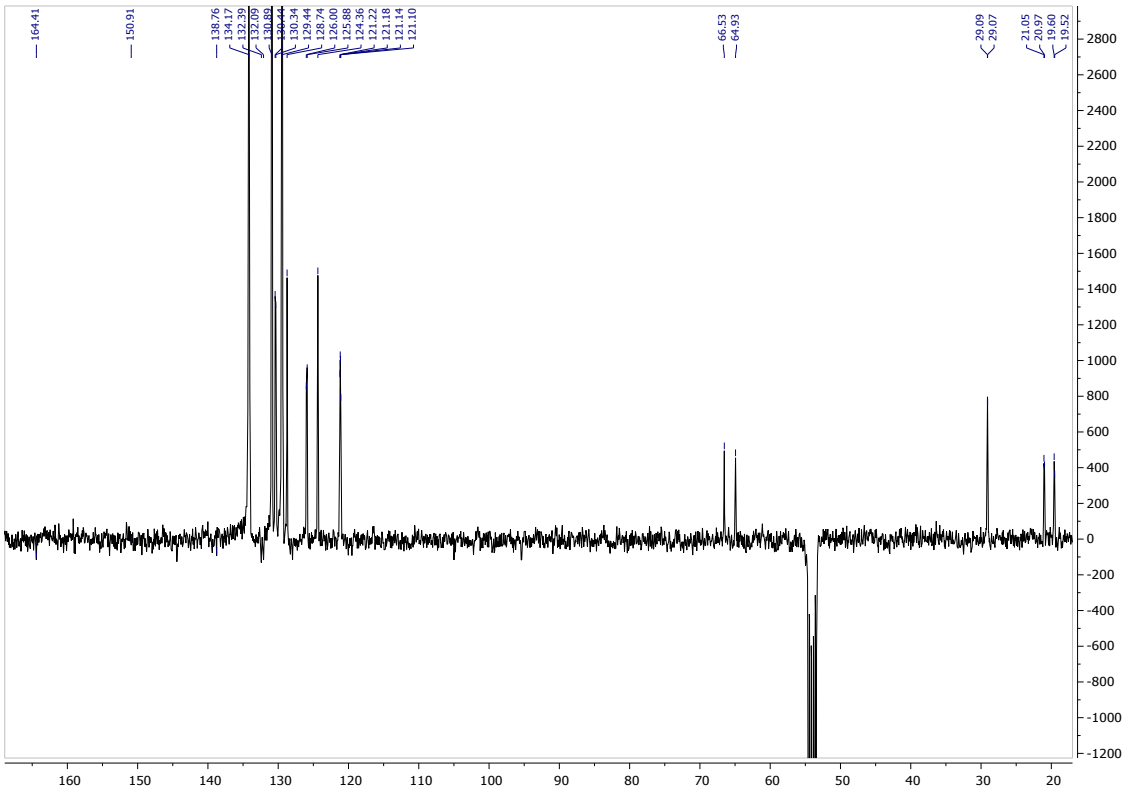


Figure S40. ^{1}HSQC spectrum of compound **[Cu(L1)(PPh$_3$)]NO$_3$ (13)**

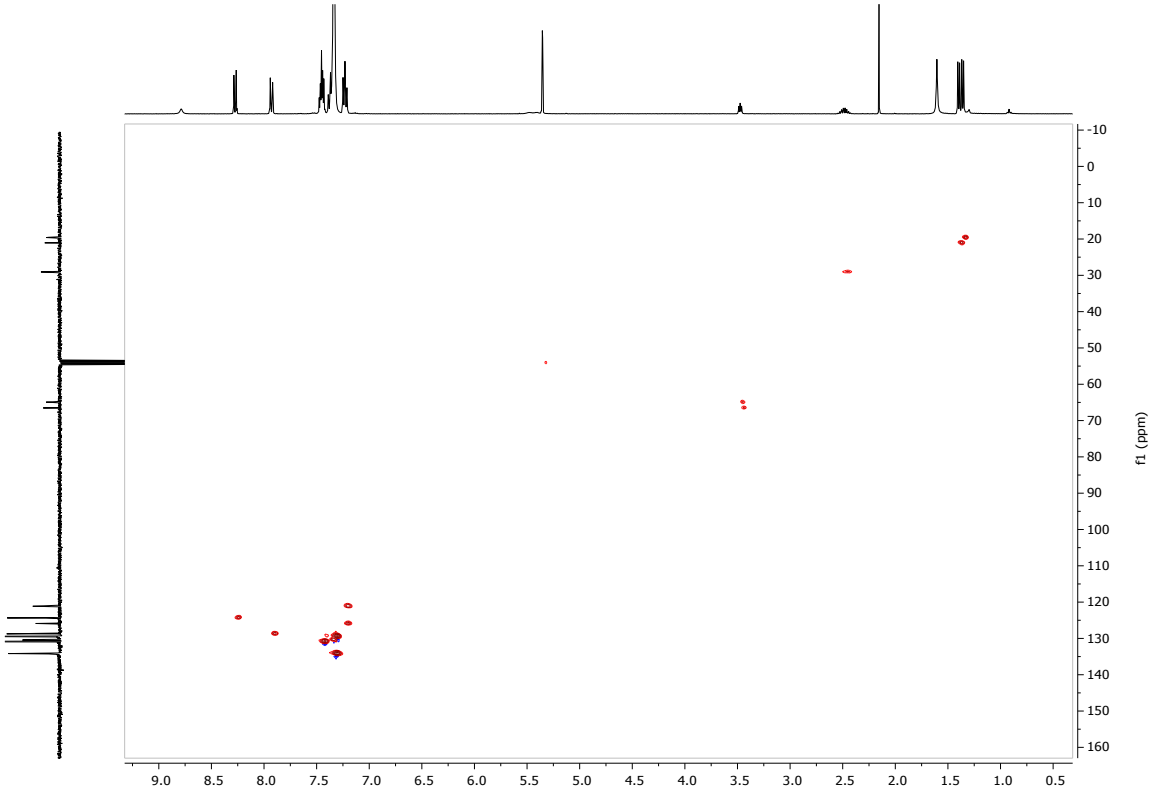
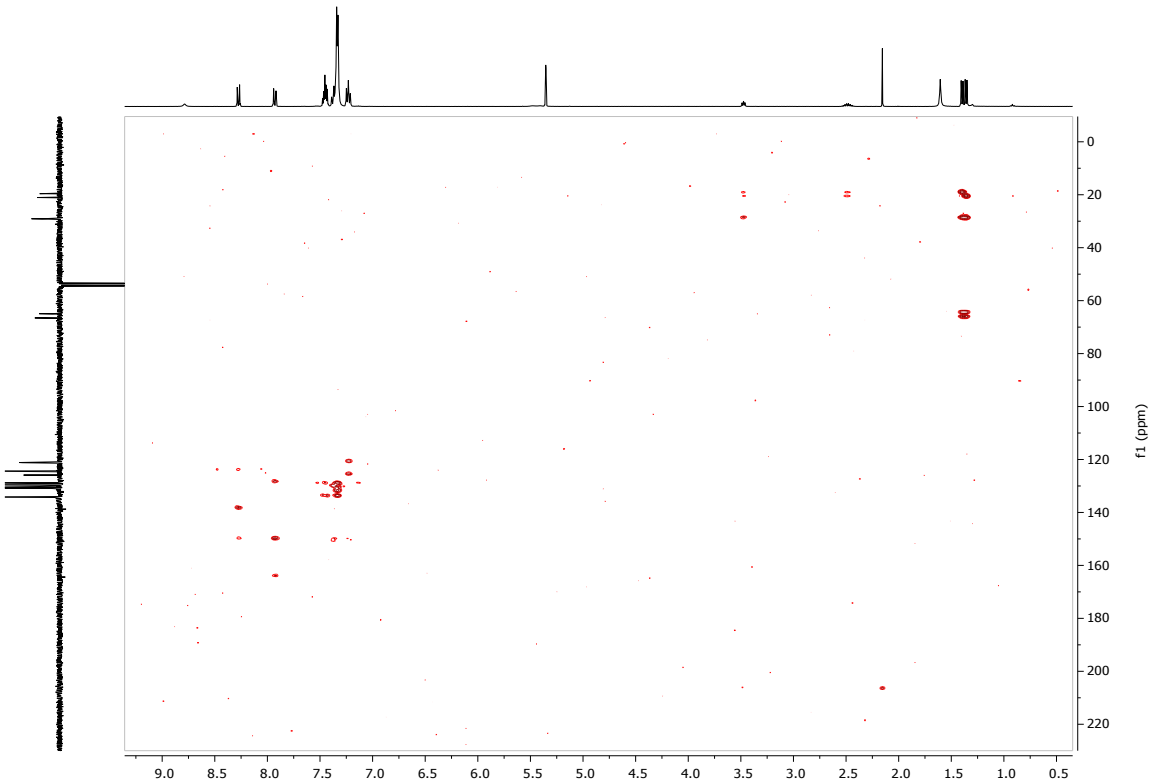


Figure S41. ^{1}HMBC spectrum of compound **[Cu(L1)(PPh$_3$)]NO$_3$ (13)**



1.14. Spectra of complex $[Cu(L2)(PPh_3)]NO_3$ (14)

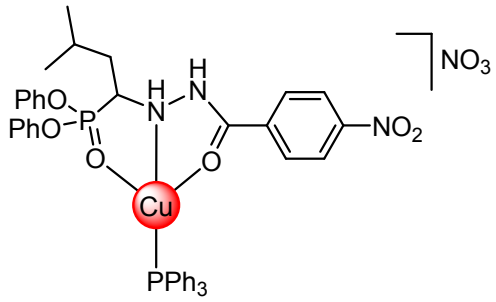


Figure S42. ^{1}H NMR spectrum of compound **$[Cu(L2)(PPh_3)]NO_3$ (14)**

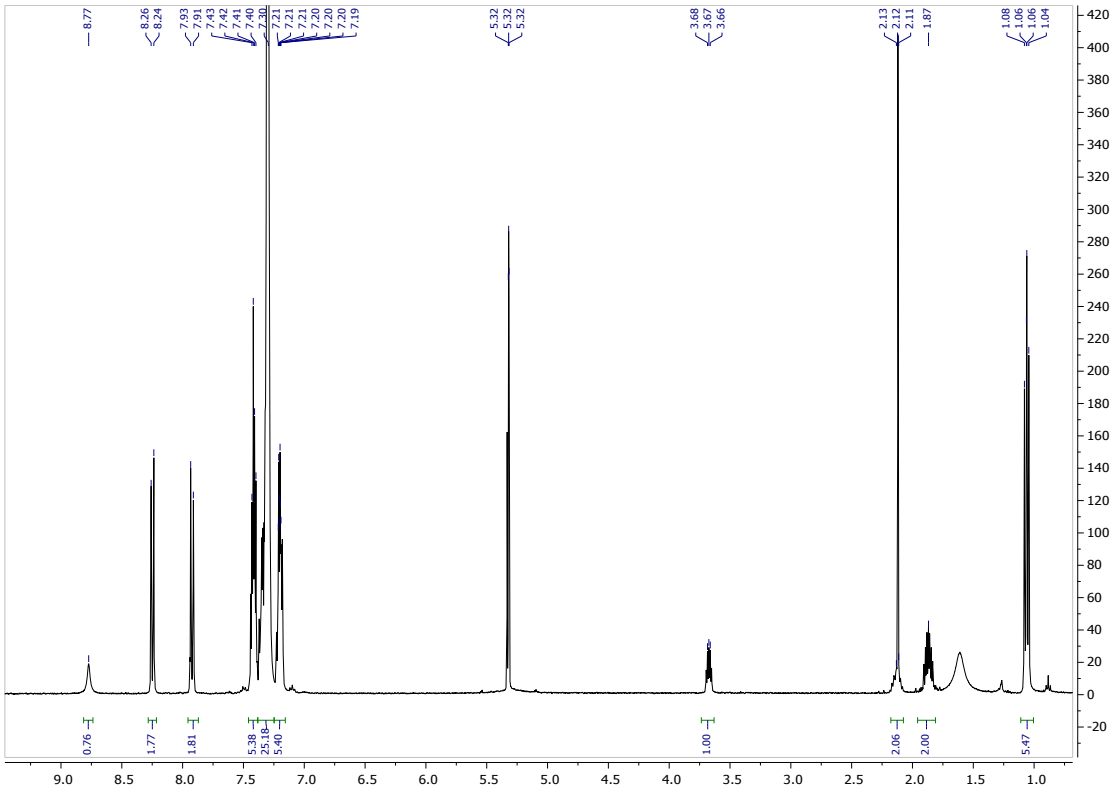


Figure S43. ^{31}P NMR spectrum of compound **[Cu(L2)(PPh$_3$)]NO$_3$ (14)**

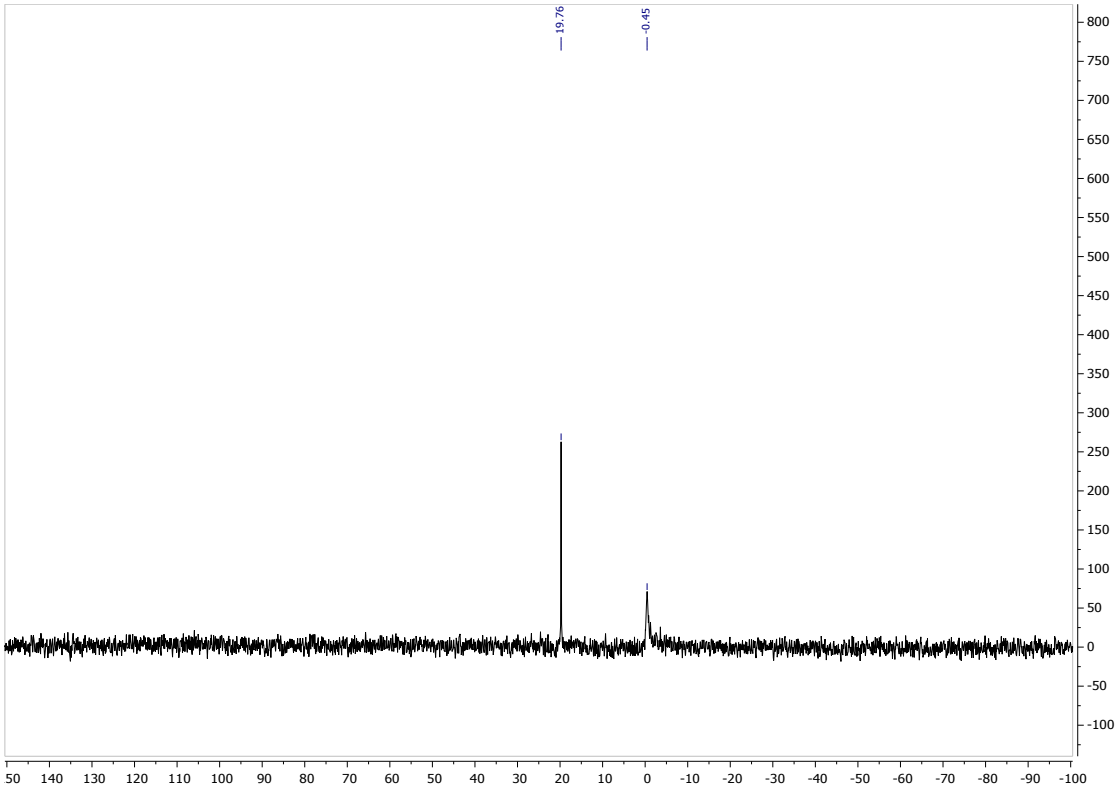


Figure S44. ^{13}C-APT spectrum of compound **[Cu(L2)(PPh$_3$)]NO$_3$ (14)**

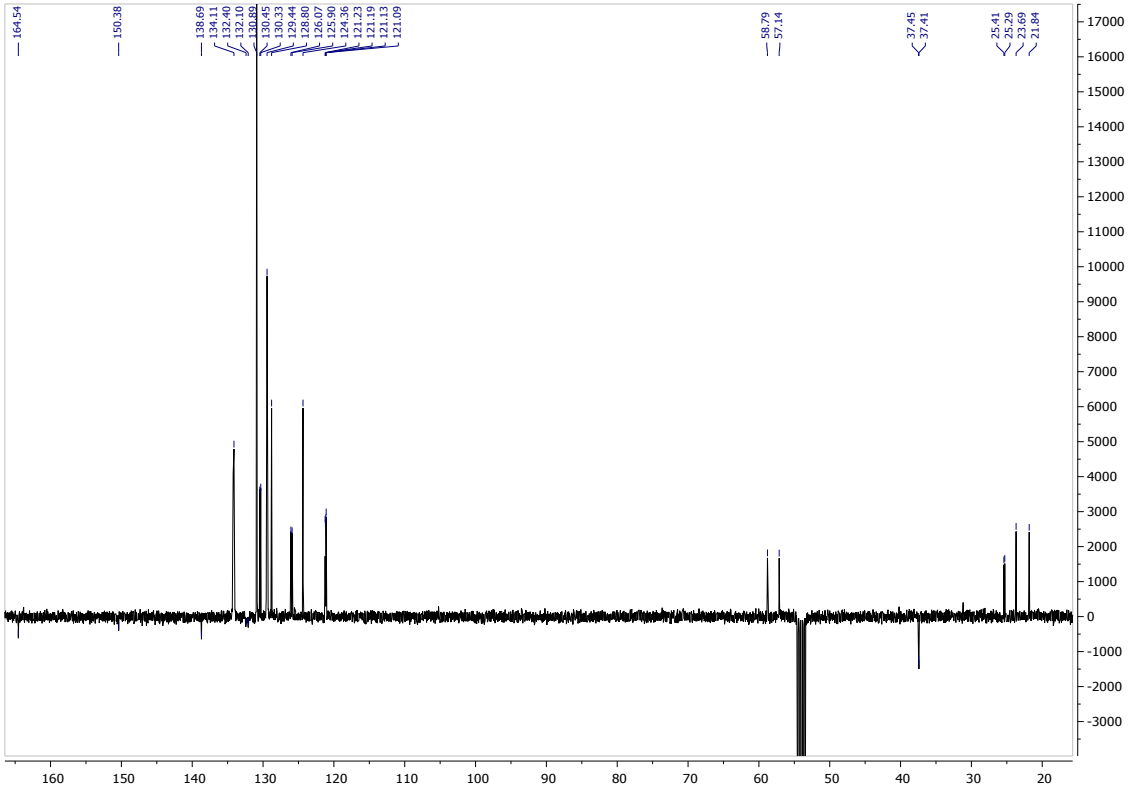


Figure S45. ^{1}HSQC spectrum of compound **[Cu(L2)(PPh$_3$)]NO$_3$ (14)**

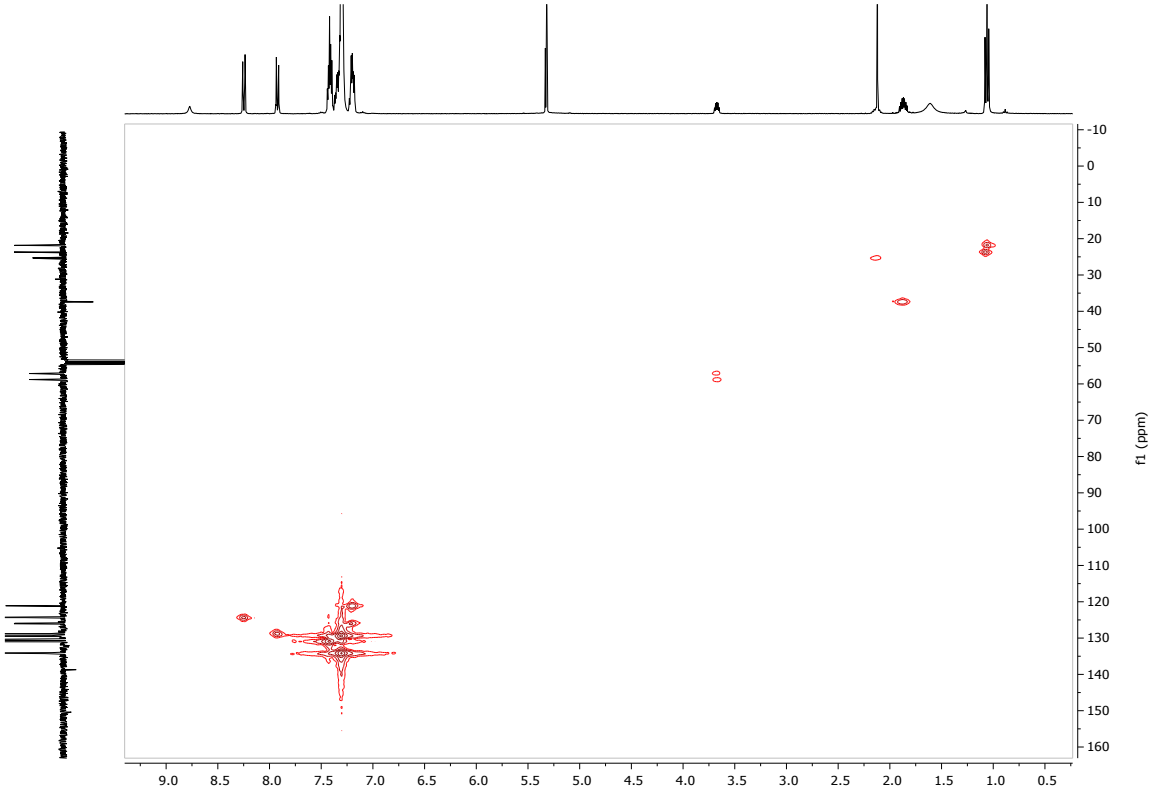
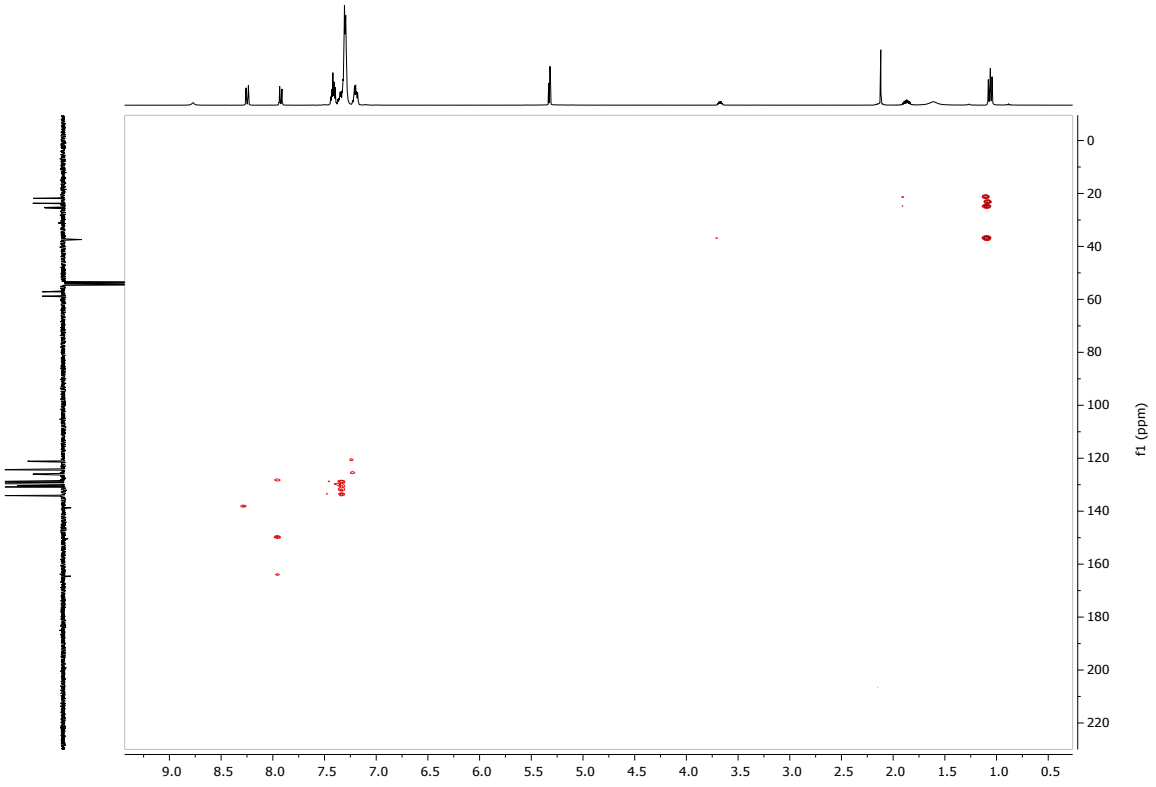


Figure S46. ^{1}HMBC spectrum of compound **[Cu(L2)(PPh$_3$)]NO$_3$ (14)**



1.15. Spectra of complex $[Cu(L3)(PPh_3)]NO_3$ (15)

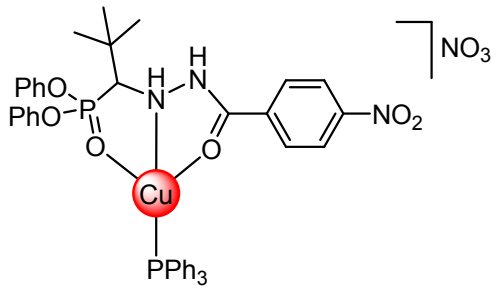


Figure S47. ^{1}H NMR spectrum of compound **$[Cu(L3)(PPh_3)]NO_3$ (15)**

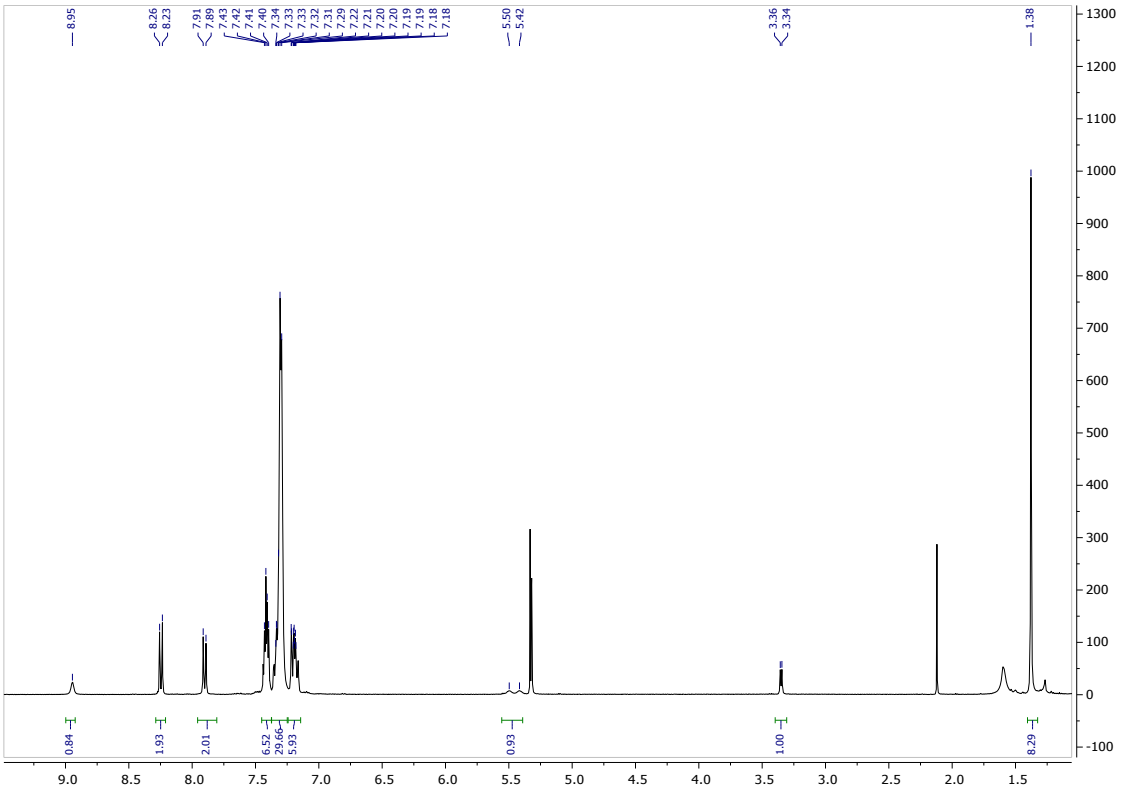


Figure S48 ^{31}P NMR spectrum of compound **[Cu(L3)(PPh$_3$)]NO$_3$ (15)**

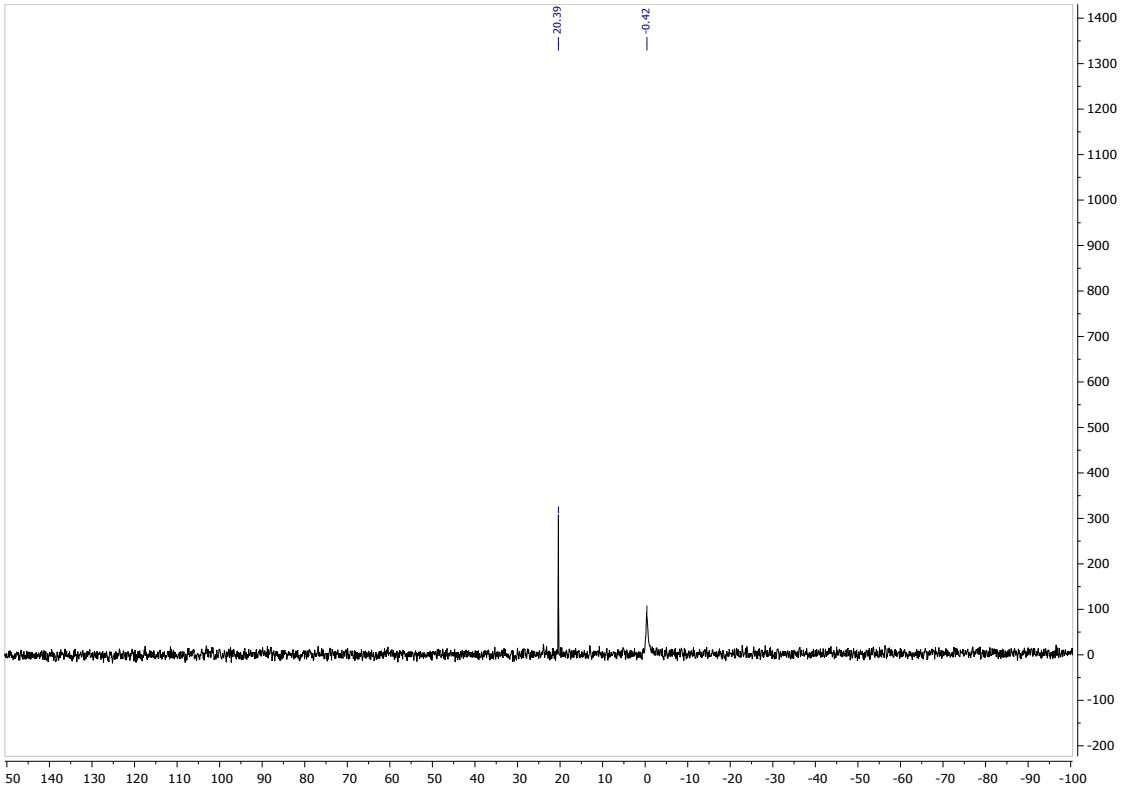


Figure S49. ^{13}C-APT spectrum of compound **[Cu(L3)(PPh$_3$)]NO$_3$ (15)**

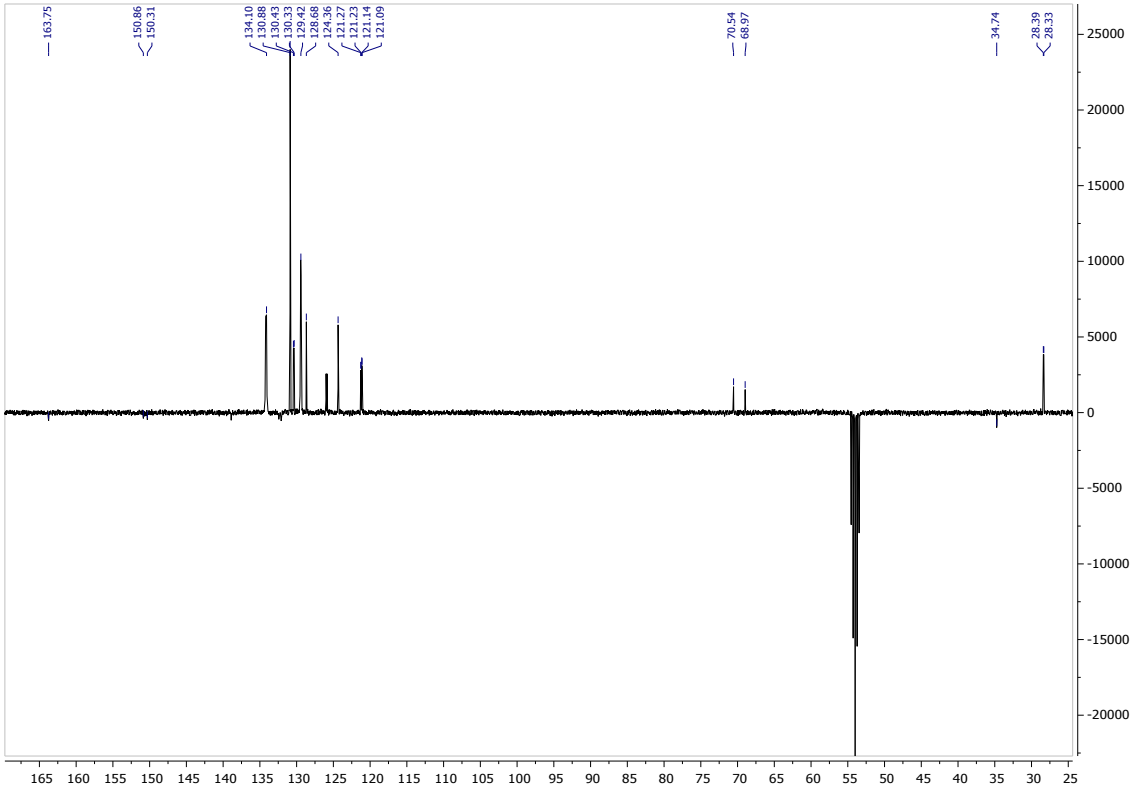


Figure S50. [1]HSQC spectrum of compound **[Cu(L3)(PPh$_3$)]NO$_3$ (15)**

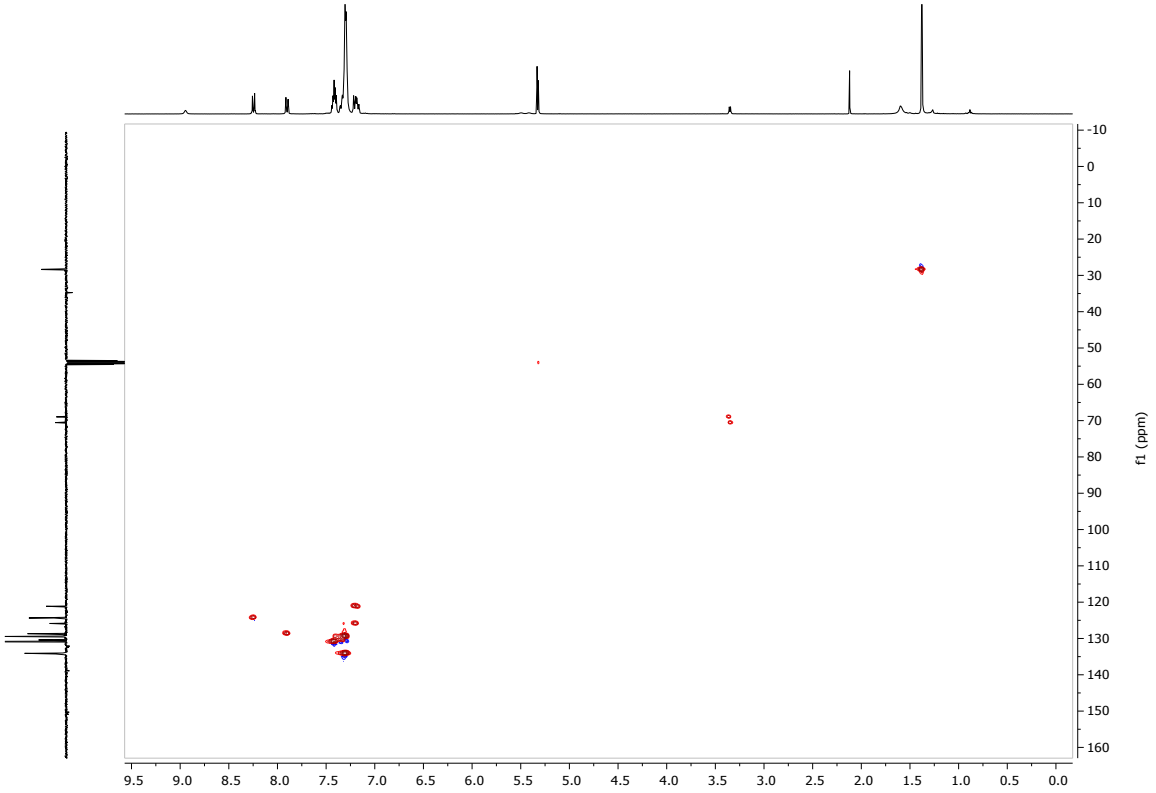
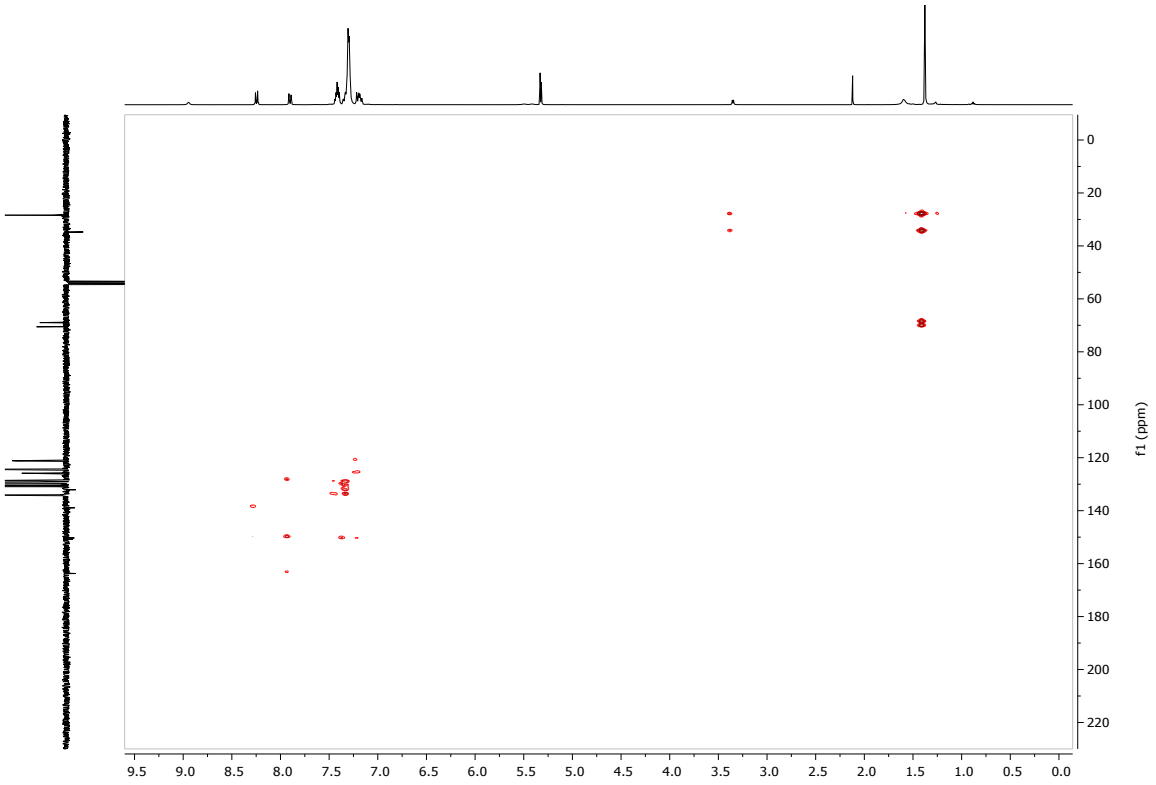


Figure S51. [1]HMBC spectrum of compound **[Cu(L3)(PPh$_3$)]NO$_3$ (15)**



1.16. Spectra of complex $[Cu(L4)(PPh_3)]NO_3$ (16)

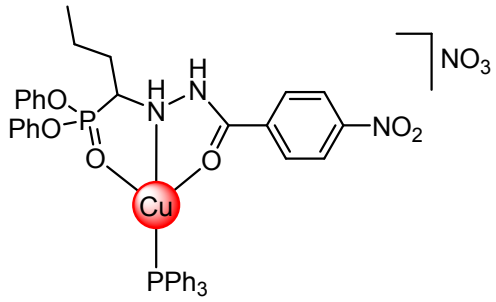


Figure S52. ^{1}H NMR spectrum of compound **$[Cu(L4)(PPh_3)]NO_3$ (16)**

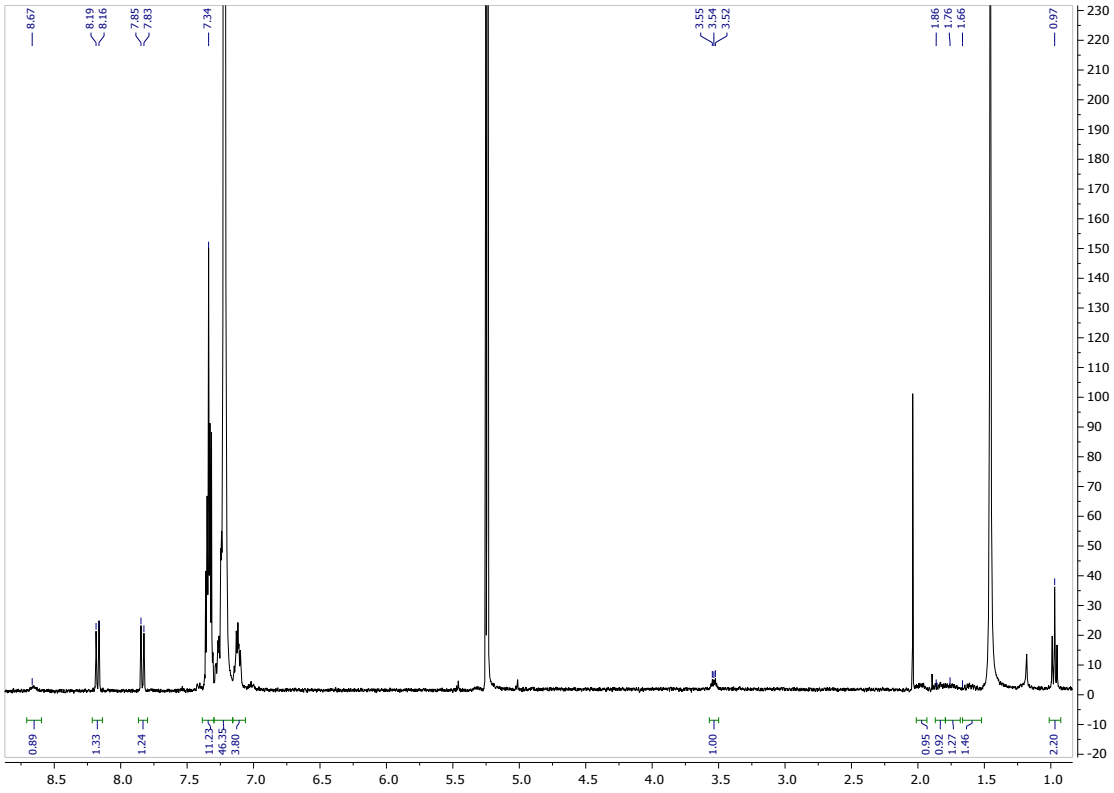
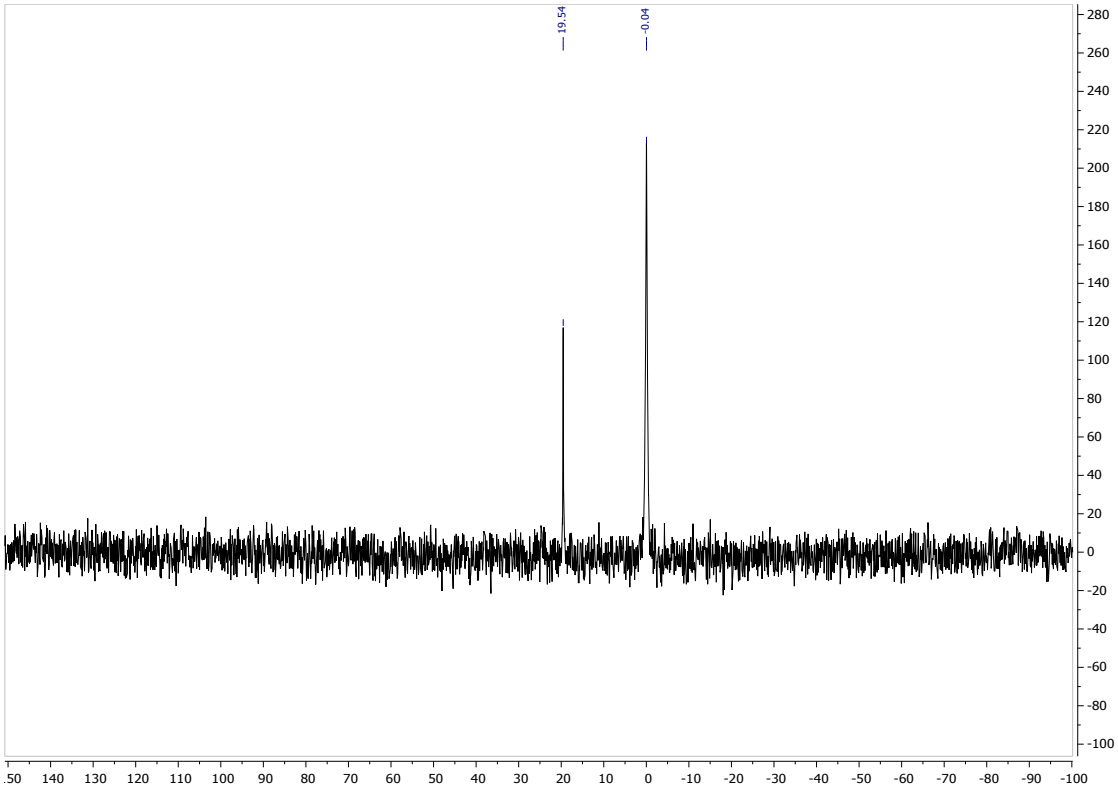


Figure S53. ^{31}P NMR spectrum of compound **[Cu(L4)(PPh$_3$)]NO$_3$ (16)**



2. X-ray data for complexes 5 and 8

2.1. Table S1. Crystal data and structure refinement for complex 5.

Identification code	c387
Empirical formula	$C_{43}H_{40}AgCl_3F_3N_3O_9P_2S$
Formula weight	1108.00
Temperature	173(2) K
Wavelength	0.71073 A
Crystal system, space group	Triclinic, P-1
Unit cell dimensions	a = 12.471(3) A alpha = 95.73(3) deg.
	b = 14.158(3) A beta = 90.95(3) deg.
	c = 14.410(3) A gamma = 105.66(3) deg.
Volume	2435.1(9) A^3
Z, Calculated density	2, 1.511 Mg/m^3
Absorption coefficient	0.753 mm^{-1}
F(000)	1124
Crystal size	0.18 x 0.14 x 0.14 mm
Theta range for data collection	4.19 to 25.50 deg.
Limiting indices	-15<=h<=15, -17<=k<=17, -17<=l<=17
Reflections collected / unique	47209 / 9030 [R(int) = 0.0566]
Completeness to theta = 25.50	99.5 %
Absorption correction	Semi-empirical from equivalents
Max. and min. transmission	0.9019 and 0.8763
Refinement method	Full-matrix least-squares on F^2
Data / restraints / parameters	9030 / 0 / 596
Goodness-of-fit on F^2	1.068
Final R indices [I>2sigma(I)]	R1 = 0.0487, wR2 = 0.1165
R indices (all data)	R1 = 0.0562, wR2 = 0.1211
Largest diff. peak and hole	1.053 and -0.869 $e.A^{-3}$

2.2. Table S2. Selected bond lengths [Å] and angles [deg] for complex 5.

Ag(1)-O(4)	2.326(2)	O(2)-C(41)	1.408(4)
Ag(1)-P(1)	2.3533(10)	C(50)-N(1)	1.490(4)
Ag(1)-O(3)	2.445(2)	N(1)-N(2)	1.411(4)
Ag(1)-N(1)	2.490(3)	N(1)-H(0)	0.86(4)
P(1)-C(11)	1.820(4)	N(2)-C(54)	1.336(4)
P(1)-C(1)	1.821(4)	N(2)-H(1)	0.80(4)
P(1)-C(21)	1.821(3)	C(54)-O(4)	1.237(4)
P(2)-O(3)	1.469(2)	C(64)-N(3)	1.469(5)
P(2)-O(1)	1.573(2)	N(3)-O(5)	1.216(4)
P(2)-O(2)	1.580(3)	N(3)-O(6)	1.218(4)
P(2)-C(50)	1.819(3)		
O(1)-C(31)	1.420(4)		

O(4)-Ag(1)-P(1)	137.79(7)	O(1)-P(2)-C(50)	100.10(14)
O(4)-Ag(1)-O(3)	84.10(9)	O(2)-P(2)-C(50)	108.90(15)
P(1)-Ag(1)-O(3)	126.92(6)	C(31)-O(1)-P(2)	122.6(2)
O(4)-Ag(1)-N(1)	69.11(8)	C(41)-O(2)-P(2)	124.5(2)
P(1)-Ag(1)-N(1)	139.69(7)	P(2)-O(3)-Ag(1)	116.27(12)
O(3)-Ag(1)-N(1)	74.57(9)	N(1)-C(50)-C(51)	111.9(3)
C(11)-P(1)-C(1)	106.03(17)	N(1)-C(50)-P(2)	106.8(2)
C(11)-P(1)-C(21)	105.17(16)	N(2)-N(1)-C(50)	111.5(2)
C(1)-P(1)-C(21)	103.88(15)	N(2)-N(1)-Ag(1)	107.37(18)
C(11)-P(1)-Ag(1)	111.27(12)	C(50)-N(1)-Ag(1)	114.73(19)
C(1)-P(1)-Ag(1)	112.89(12)	N(2)-N(1)-H(0)	104(2)
C(21)-P(1)-Ag(1)	116.70(11)	O(5)-N(3)-O(6)	123.4(3)
O(3)-P(2)-O(1)	116.52(14)	O(5)-N(3)-C(64)	118.2(3)
O(3)-P(2)-O(2)	114.13(14)	O(6)-N(3)-C(64)	118.4(3)
O(1)-P(2)-O(2)	101.19(13)		
O(3)-P(2)-C(50)	114.38(14)		

2.3. Table S3. Crystal data and structure refinement for complex 8.

Identification code	c404
Empirical formula	$C_{42}H_{39}AgF_3N_3O_9P_2S$
Formula weight	988.63
Temperature	100(2) K
Wavelength	0.71073 A
Crystal system, space group	Triclinic, P-1
Unit cell dimensions	a = 13.114(3) A alpha = 89.03(3) deg.
	b = 15.701(3) A beta = 88.03(3) deg.
	c = 21.412(4) A gamma = 78.01(3) deg.
Volume	4309.8(15) A^3
Z, Calculated density	4, 1.524 Mg/m^3
Absorption coefficient	0.661 mm^{-1}
F(000)	2016
Crystal size	0.40 x 0.08 x 0.06 mm
Theta range for data collection	4.17 to 25.50 deg.
Limiting indices	-15<=h<=15, -19<=k<=19, -25<=l<=25
Reflections collected / unique	63598 / 15933 [R(int) = 0.0871]
Completeness to theta = 25.50	99.5 %
Absorption correction	Semi-empirical from equivalents
Max. and min. transmission	0.9614 and 0.7778
Refinement method	Full-matrix least-squares on F^2
Data / restraints / parameters	15933 / 6 / 1110
Goodness-of-fit on F^2	1.051
Final R indices [I>2sigma(I)]	R1 = 0.0890, wR2 = 0.1971
R indices (all data)	R1 = 0.1322, wR2 = 0.2193
Largest diff. peak and hole	3.957 and -1.320 $e.A^{-3}$

2.4. Table S4. Selected bond lengths [Å] and angles [deg] for complex 8.

Ag(1)-O(4)	2.348(5)	Ag(2)-O(10)	2.321(5)
Ag(1)-P(1)	2.352(2)	Ag(2)-P(3)	2.345(2)
Ag(1)-N(1)	2.447(5)	Ag(2)-N(4)	2.404(6)
Ag(1)-O(3)	2.471(5)	P(3)-C(71)	1.788(8)
P(1)-C(11)	1.812(8)	P(3)-C(81)	1.833(8)
P(1)-C(1)	1.812(8)	P(3)-C(61)	1.836(8)
P(1)-C(21)	1.826(8)	P(4)-O(9)	1.468(5)
P(2)-O(3)	1.467(5)	P(4)-O(7)	1.575(5)
P(2)-O(1)	1.580(5)	P(4)-O(8)	1.585(5)
P(2)-O(2)	1.588(5)	P(4)-C(87)	1.807(7)
P(2)-C(37)	1.812(7)	N(4)-N(5)	1.426(8)
N(1)-N(2)	1.430(8)	N(4)-C(87)	1.482(9)
N(1)-C(37)	1.481(8)	N(5)-C(107)	1.335(9)
N(2)-C(47)	1.340(9)	N(6)-O(11)	1.229(8)
N(3)-O(5)	1.222(8)	N(6)-O(12)	1.237(8)
N(3)-O(6)	1.239(8)	N(6)-C(114)	1.463(9)
N(3)-C(54)	1.474(9)	O(7)-C(91)	1.401(9)
O(1)-C(31)	1.401(9)	O(8)-C(101)	1.404(8)
O(2)-C(41)	1.410(8)	O(10)-C(107)	1.226(8)
O(4)-C(47)	1.235(8)		

O(4)-Ag(1)-P(1)	137.97(13)	P(2)-O(3)-Ag(1)	113.6(3)
O(4)-Ag(1)-N(1)	69.68(17)	C(47)-O(4)-Ag(1)	115.9(4)
P(1)-Ag(1)-N(1)	144.18(15)	O(10)-Ag(2)-P(3)	136.57(13)
O(4)-Ag(1)-O(3)	86.12(17)	O(10)-Ag(2)-N(4)	71.65(18)
P(1)-Ag(1)-O(3)	119.64(12)	P(3)-Ag(2)-N(4)	150.40(15)
N(1)-Ag(1)-O(3)	76.08(17)	C(71)-P(3)-C(81)	104.4(4)
C(11)-P(1)-C(1)	102.6(4)	C(71)-P(3)-C(61)	105.0(4)
C(11)-P(1)-C(21)	107.1(3)	C(81)-P(3)-C(61)	106.0(3)
C(1)-P(1)-C(21)	107.8(4)	C(71)-P(3)-Ag(2)	117.2(3)
C(11)-P(1)-Ag(1)	114.8(3)	C(81)-P(3)-Ag(2)	110.3(2)
C(1)-P(1)-Ag(1)	113.7(3)	C(61)-P(3)-Ag(2)	113.0(3)
C(21)-P(1)-Ag(1)	110.2(3)	O(9)-P(4)-O(7)	116.9(3)
O(3)-P(2)-O(1)	115.5(3)	O(9)-P(4)-O(8)	115.1(3)
O(3)-P(2)-O(2)	114.5(3)	O(7)-P(4)-O(8)	101.4(3)
O(1)-P(2)-O(2)	102.0(3)	O(9)-P(4)-C(87)	115.0(3)
O(3)-P(2)-C(37)	114.8(3)	O(7)-P(4)-C(87)	100.6(3)
O(1)-P(2)-C(37)	101.8(3)	O(8)-P(4)-C(87)	105.9(3)
O(2)-P(2)-C(37)	106.7(3)	N(5)-N(4)-C(87)	111.1(6)
N(2)-N(1)-C(37)	112.1(5)	N(5)-N(4)-Ag(2)	107.1(4)
N(2)-N(1)-Ag(1)	107.7(3)	C(87)-N(4)-Ag(2)	116.2(4)
C(37)-N(1)-Ag(1)	114.5(4)	C(107)-N(5)-N(4)	121.0(6)
C(47)-N(2)-N(1)	120.4(5)	O(11)-N(6)-O(12)	123.0(6)
O(5)-N(3)-O(6)	123.7(6)	O(11)-N(6)-C(114)	118.3(6)
O(5)-N(3)-C(54)	117.2(6)	O(12)-N(6)-C(114)	118.7(6)
O(6)-N(3)-C(54)	119.1(6)	C(91)-O(7)-P(4)	122.6(4)
C(31)-O(1)-P(2)	121.2(4)	C(101)-O(8)-P(4)	125.0(4)
C(41)-O(2)-P(2)	124.3(4)	C(107)-O(10)-Ag(2)	114.8(4)