Free-Catalysed Synthesis of Thiazolidine-Thiourea Ligands for Metal Coordination (Au and Ag) and Preliminary Cytotoxic Studies

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1. NMR spectra of 2-amino-2-thiazolines and 2-iminothiazolidines

Figure S1. ¹H NMR (300 MHz, CDCl₃) spectrum of compound 4.



Figure S3. ¹H NMR (400 MHz, CDCl₃) spectrum of compound 5.



Figure S4. ¹³C{¹H} APT NMR (101 MHz, CDCl₃) spectrum of compound 5.



Figure S5. ¹H NMR (400 MHz, CDCl₃) spectrum of compound 6.



Figure S6. ¹³C{¹H} APT NMR (101 MHz, CDCl₃) spectrum of compound 6.



Figure S7. ¹H NMR (400 MHz, CDCl₃) spectrum of compound 7.



Figure S8. ¹³C{¹H} APT NMR (101 MHz, CDCl₃) spectrum of compound 7.



Figure S9. ¹⁹F NMR (376 MHz, CDCl₃) spectrum of compound 7.



Figure S10. ¹H NMR (400 MHz, CDCl₃) spectrum of compound 8.







Figure S12. ¹⁹F NMR (376 MHz, CDCl₃) spectrum of compound 8.





Figure S13. ¹H NMR (400 MHz, CDCl₃) spectrum of compound 9.





Figure S15. ¹⁹F NMR (376 MHz, CDCl₃) spectrum of compound 9.



111.2 -111.4 -111.6 -111.8 -112.0 -112.2 -112.4 -112.6 -112.8 -113.0 -113.2 -113.4 -113.6 -113.8 -114.0 -114.4 -114.4 -114.6 -114. ppm

2. NMR spectra of thiazolidine-thioureas 10-12

Figure S16. ¹H NMR (400 MHz, (CD₃)₂CO) spectrum of compound 10.



Figure S17. ${}^{13}C{}^{1}H$ APT NMR (101 MHz, (CD₃)₂CO) spectrum of compound 10.



Figure S18. ¹H NMR (400 MHz, (CD₃)₂CO) spectrum of compound 11.





Figure S19. ${}^{13}C{}^{1}H$ APT NMR (101 MHz, (CD₃)₂CO) spectrum of compound 11.

Figure S20. ¹⁹F NMR (376 MHz, CDCl₃) spectrum of compound 11.





Figure S21. ¹H NMR (400 MHz, (CD₃)₂CO) spectrum of compound 12.

Figure S22. ${}^{13}C{}^{1}H$ APT NMR (101 MHz, (CD₃)₂CO) spectrum of compound 12.



2. NMR spectra of silver complexes 13-18

Figure S23. ¹H NMR (400 MHz, (CD₃)₂CO) spectrum of complex 13.



Figure S24. ${}^{13}C{}^{1}H$ APT NMR (101 MHz, (CD₃)₂CO) spectrum of complex 13.



Figure S25. ${}^{31}P{}^{1}H$ NMR (162 MHz, (CD₃)₂CO) spectrum of complex 13.



30 20 f1 (ppm) 10

0

-10

-20 -30

-40 -50

-60 -70 -80

-90 -10

— 12.0



70 60

50

40

90 80

150 140 130 120 110 100



Figure S27. ${}^{13}C{}^{1}H$ APT NMR (101 MHz, (CD₃)₂CO) spectrum of complex 14.



Figure S28. 19 F NMR (376 MHz, (CD₃)₂CO) spectrum of complex 14.



Figure S29. ${}^{31}P{}^{1}H$ NMR (162 MHz, (CD₃)₂CO) spectrum of complex 14.



Figure S30. ¹H NMR (400 MHz, (CD₃)₂CO) spectrum of complex 15.



Figure S31. ${}^{13}C{}^{1}H$ APT NMR (101 MHz, (CD₃)₂CO) spectrum of complex 15.



Figure S32. ${}^{31}P{}^{1}H$ NMR (ppm) (162 MHz, (CD₃)₂CO) spectrum of complex 15.



Figure S33. ¹H NMR (400 MHz, (CD₃)₂CO) spectrum of complex 16.



Figure S34. ${}^{13}C{}^{1}H$ APT NMR (101 MHz, (CD₃)₂CO) spectrum of complex 16.



Figure S35. ¹H NMR (400 MHz, (CD₃)₂CO) spectrum of complex 17.



Figure 37. ¹⁹F NMR (376 MHz, (CD₃)₂CO) spectrum of complex 17.





Figure S39. ${}^{13}C{}^{1}H$ APT NMR (101 MHz, (CD₃)₂CO) spectrum of complex 18.

3. NMR spectra of gold complexes 19-27

Figure S40. ¹H NMR (400 MHz, (CD₃)₂CO) spectrum of complex 19.



Figure S42. ${}^{31}P{}^{1}H$ NMR (162 MHz, (CD₃)₂CO) spectrum of complex 19.



Figure S43. ¹H NMR (400 MHz, (CD₃)₂CO) spectrum of complex 20.



Figure S44. ${}^{13}C{}^{1}H$ APT NMR (101 MHz, (CD₃)₂CO) spectrum of complex 20.



Figure S45. ¹⁹F NMR (376 MHz, (CD₃)₂CO) spectrum of complex 20.



Figure S46. ${}^{31}P{}^{1}H$ NMR (162 MHz, (CD₃)₂CO) spectrum of complex 20.



Figure S47. ¹H NMR (400 MHz, (CD₃)₂CO) spectrum of complex 21.



Figure S48. ${}^{13}C{}^{1}H$ APT NMR (101 MHz, (CD₃)₂CO) spectrum of complex 21.



Figure S50. ¹H NMR (400 MHz, (CD₃)₂CO) spectrum of complex 22.



Figure S51. ${}^{13}C{}^{1}H$ APT NMR (101 MHz, (CD₃)₂CO) spectrum of complex 22.



Figure S52. ${}^{19}F{}^{1}H$ NMR (376 MHz, (CD₃)₂CO) spectrum of complex 22.



Figure S53. ¹H NMR (400 MHz, (CD₃)₂CO) spectrum of complex 23.



Figure S54. ${}^{13}C{}^{1}H$ APT NMR (101 MHz, (CD₃)₂CO) spectrum of complex 23.



Figure S55. ${}^{19}F{}^{1}H$ NMR (376 MHz, (CD₃)₂CO) spectrum of complex 23.



-66 -68 -70 -72 -74 -76 -78 -80 -82 -84 -86 -88 -90 -92 -94 -96 -98 -100 -102 -104 -106 -108 -110 -112 -114 -116 -118 -120

Figure S56. ¹H NMR (400 MHz, (CD₃)₂CO) spectrum of complex 24.



Figure S57. ${}^{13}C{}^{1}H$ APT NMR (101 MHz, (CD₃)₂CO) spectrum of complex 24.



Figure S58. ${}^{19}F{}^{1}H$ NMR (376 MHz, (CD₃)₂CO) spectrum of complex 24.



Figure S59. ¹H NMR (400 MHz, (CD₃)₂CO) spectrum of complex 25.



Figure S60. ${}^{13}C{}^{1}H$ APT NMR (101 MHz, (CD₃)₂CO) spectrum of complex 25.



Figure S61. ¹⁹F NMR (ppm) (376 MHz, (CD₃)₂CO spectrum of complex 25.



Figure S62. ¹H NMR (400 MHz, (CD₃)₂CO) spectrum of complex 26.



Figure S63. ${}^{13}C{}^{1}H$ APT NMR (101 MHz, (CD₃)₂CO) spectrum of complex 26.



-112 -114 -116 -118 -120 -122 -124 -126 -128 -130 -132 -134 -136 -138 -140 -142 -144 -146 -148 -150 -152 -154 -156 -158 -160 -162 -164 -166 -168 -170 -172 f1 (ppm)

Figure S65. ¹H NMR (400 MHz, (CD₃)₂CO) spectrum of complex 27.



Figure S67. ¹⁹F NMR (376 MHz, (CD₃)₂CO spectrum of complex 27.



-105	-110	-115	-120	-125	-130	-135	-140	-145	-150	-155	-160	-165	-17() -175
							f1 (ppm)							