Electronic Supplementary Material (ESI) for Medicinal Chemistry Communications

Supporting Information

TrxR Inhibition and Antiproliferative Activities of Structurally Diverse Gold *N*-Heterocyclic Carbene Complexes

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Full crystallographic and refinement parameters as well as tables with bond distances and angles

Tab S1.: selected bond distances (Å) and angles (°) for **1f**

Atoms	Bond distances (Å)	Atoms	Bond angles (°)
C1-Au1	2.013(4)	C1-Au1-S1	175.1(1)
S1-Au1	2.302(1)	C17-S1-Au1	101.2(2)
C1-N1	1.343(6)	N1-C1-Au1	127.8(3)
C1-N2	1.358(5)	N2-C1-Au1	126.4(3)
S1-C17	1.792(5)	N1-C1-N2	105.5(4)
C16-O1	1.391(7)		
Au1-Au1*	3.2688(2)		

Tab S2.: Crystal data and structure refinement for **1f**

Empirical formula	$C_{26}H_{27}N_2OSAu$
Formula weight[g/mol]	612.52
Color and shape	Colorless needles
Crystal system	Triclinic
Space group	P-1
Crystal size [mm3]	0.11 x 0.03 x 0.02
a [Å]	9.7700(2)
b [Å]	9.7877(3)
c [Å]	12.2436(5)
α [°]	88.650(3)
β [°]	87.135(3)
γ [°]	75.316(2)
Volume [$Å^3$]	1131.09(6)
Temperature [K]	150
Z	2
μ [mm^{-1}]	6.617
ρ_{calc} [g/cm^3]	1.798
Theta range for data collection [°]	3.1752 - 58.6592
Reflections collected	9021
Independent reflections	5206[R(int)=0.0245]
Final R indexes [I>2σ (I)]	0.0315
Final R indexes [all data]	wR_2 0.0652
Goodness-of-fit on F^2	1.107
Largest diff. peak/hole [e/$Å^3$] min/max	1.864 / -2.156
CCDC deposition code	927677