

Supporting Information for the article ‘Synthesis, crystal structures, and *in vitro* anticancer properties of new *N*-heterocyclic carbene (NHC) silver(I)- and gold(I)/(III)-complexes: A rare example of silver(I)-NHC complex involved in redox transmetallation’

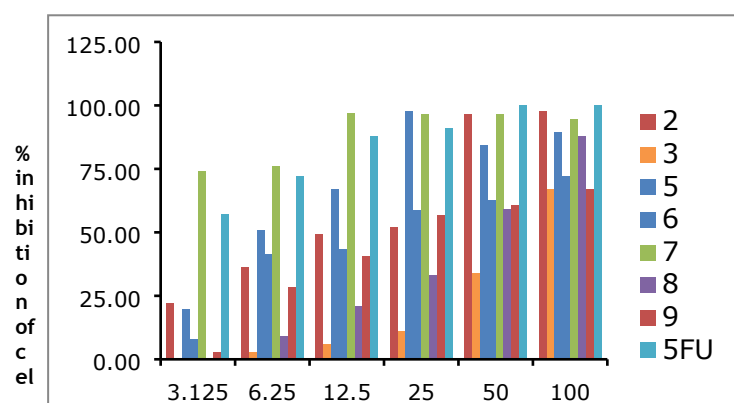
22nd July 2016

Note added after first publication: The CCDC crystal structure data file for this article, originally published on 23rd June 2016, has been replaced. For further detail, please view the Correction addendum for this article.

Table S1. Crystal data and structure refinement details for compounds **5a**, **6**, **7**, and **8**.

	5a	6	7	8
Formula	C ₂₂ H ₂₈ N ₄ AgPF ₆	C ₃₇ H ₃₅ N ₅ AgBr	C ₁₅ H ₁₇ N ₄ AuCl ₃	C ₂₂ H ₃₂ N ₄ O ₂ AuCl
Formula weight	601.32	697.19	542.63	616.93
Crystal system	Monoclinic	Triclinic	Monoclinic	Monoclinic
Space group	C2/c	<i>P</i> 1	<i>P</i> 21/c	<i>P</i> 21/c
Unit cell dimensions				
a (Å)	20.1752(4)	10.5279(2)	16.5289(7)	7.5995(8)
b (Å)	7.1076(2)	10.7966(3)	8.5610(3)	19.115(2)
c (Å)	16.9290(4)	14.6437(2)	14.5774(6)	15.8809(18)
α (°)	90.00	108.4830(10)	90.00	90.00
β (°)	96.6190(10)	91.926(2)	113.8300(10)	95.730(3)
γ (°)	90.00	100.9250(10)	90.00	90.00
V (Å ³)	2411.39(10)	1542.15(6)	1886.90(13)	2295.5(4)
Z	4	2	4	4
Density (calcd) (gm/cm ³)	1.656	1.501	1.910	1.785

Abs coeff (mm ⁻¹)	0.967	0.698	8.220	6.551
F(000)	1216	717	1032	1216
Crystal size (mm)	0.40 × 0.23 × 0.08	0.39 × 0.25 × 0.13	0.34 × 0.14 × 0.14	0.58 × 0.05 × 0.03
Temperature (K)	100	100	100	100
Radiation (Å)	MoKa 0.71073	MoKa 0.71073	MoKa 0.71073	MoKa 0.71073
θ Min, max (°)	2.03, 32.70	1.98, 30.12	1.35, 32.65	1.67, 29.99
Dataset	-30:30;-10:10;-25:23	-14:14;-15:15;-20:20	-24:25;-12:12;-22:18	-10:10;-26:26;-22:22
Tot.; Uniq. Data	28427	32999	25380	6583
R (int)	0.0371	0.0253	0.0238	0.0725
Nref, Npar	4411, 158	8981, 340	6791, 196	5215, 276
R, wR ₂ , S	0.0468, 0.0682, 1.21	0.1683, 0.3752, 2.37	0.0758, 0.2514, 1.15	0.0650, 0.1524, 1.14



Concentrations of test sample in μM

Figure S1. Effects of increasing amounts of salts and carbene complexes on the percentage inhibition of HCT 116 cell proliferation.

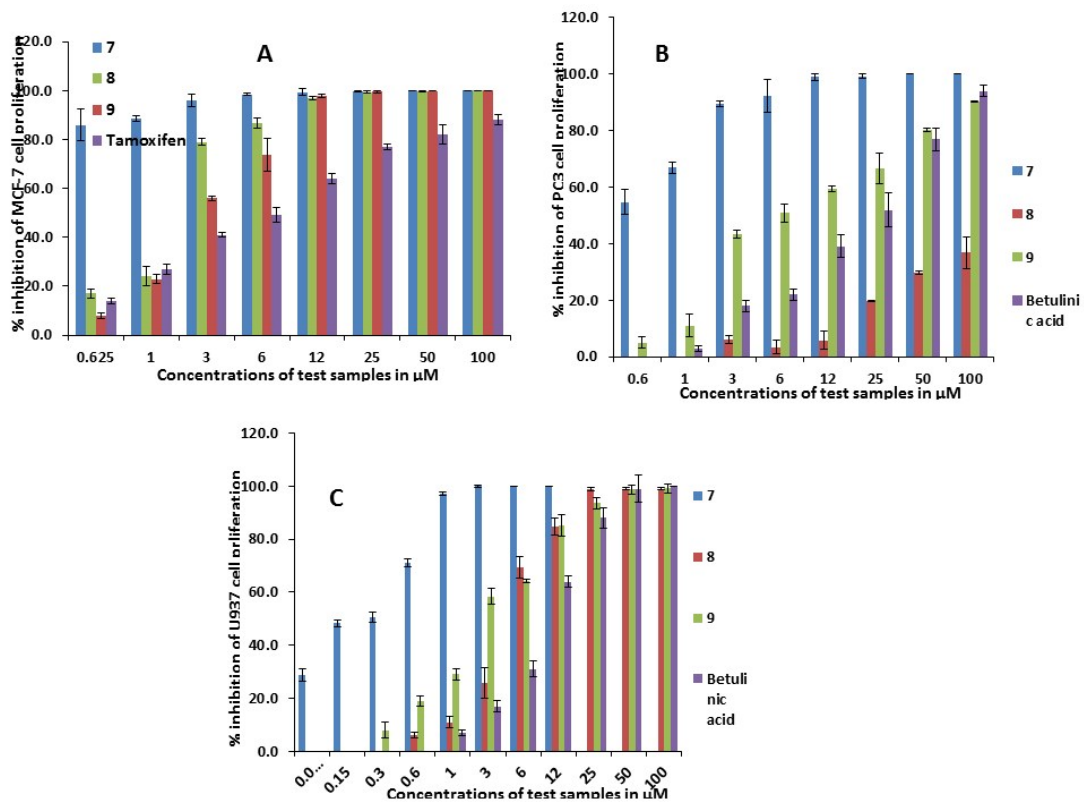


Figure S2. Effects of increasing amounts of Au-carbene complexes on the percentage inhibition of MCF-7 (A), PC3 (B), and U937(C) cell proliferation.