Supporting Information for

Dinuclear gold(I) complexes with pyrimidine- and *m*-carborane-based bisphosphine ligands: synthesis, structure, photoluminescence and cytotoxicity against malignant pleural mesothelioma

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Table S1. Crystal data and structure refinement for **Au1** and **Au2**·1.8CH_2Cl_2

	Au1	**Au2**·1.8CH_2Cl_2
Chemical formula	$C_{28}H_{22}Au_2Cl_2N_2P_2$	$C_{61.8}H_{79.6}Au_4B_{20}C_{l7.6}P_4$
M_r	913.25	2219.96
Crystal system, space group	Triclinic, *P* 1	Monoclinic, *C*2/*c*
a, *b*, *c* (Å)	9.2240 (2), 13.7796 (3), 21.7778 (4)	32.1688 (10), 13.7076 (4), 18.0035 (6)
α, β, γ (°)	94.548 (1), 91.601 (1), 90.471 (1)	90, 102.182 (1), 90
V (Å^3)	2758.08 (10)	7760.0 (4)
μ (mm^{-1})	10.96	7.87
Crystal size (mm)	0.20 × 0.20 × 0.15	0.20 × 0.20 × 0.08
T_{min}, T_{max}	0.422, 0.746	0.479, 0.746
No. of measured, independent and observed [$I > 2\sigma(I)$] reflections	51948, 16837, 14870	48239, 10914, 8991
R_{int}	0.045	0.034
$(\sin\theta/\lambda)_{max}$ (Å^{-1})	0.715	0.695
Range of *h*, *k*, *l*	*h* = -13→13, *k* = -19→19, *l* = -31→31	*h* = -41→44, *k* = -19→19, *l* = -24→25
$R[F^2 > 2\sigma(F^2)]$, $wR(F^2)$, *S*	0.030, 0.073, 1.07	0.031, 0.073, 1.03
No. of reflections	16837	10914
No. of parameters	750	563
No. of restraints	739	564
Weighting scheme	$w = 1/[\sigma^2(F_o^2) + 0.8746P]$ where $P = (F_o^2 + 2F_c^2)/3$	$w = 1/[\sigma^2(F_o^2) + (0.0259P)^2 + 44.2983P]$ where $P = (F_o^2 + 2F_c^2)/3$
$\Delta\rho_{max}$, $\Delta\rho_{min}$ (e Å^{-3})	1.58, -2.15	3.43, -1.86

Computer programs: *APEX3* (Bruker-AXS, 2016), *SAINT* (Bruker-AXS, 2016), *SHELXT* 2018/2 (Sheldrick, 2018), *SHELXL2019*/2 (Sheldrick, 2019), *ShelXle* (Hübschle, 2011), *enCIFer* (Allen *et al.*, 2004).

Table S2. Selected geometric parameters for crystal structures of **Au1** and **Au2**·1.8CH_2Cl_2

Au1			
Distances, Å			
P2—Au2B (1)	2.3068 (10)	Cl3B—Au3B (2)	2.280 (8)
P2—Au2A (1)	2.1629 (9)	Cl3A—Au3A (2)	2.299 (8)
Au1—Cl1 (1)	2.2831 (10)	Au4—Cl4 (2)	2.2835 (9)
Au2B—Cl2B (1)	2.3035 (16)	Au3B—P3B (2)	2.241 (8)
Au2A—Cl2A (1)	2.2987 (16)	Au3A—P3A (2)	2.217 (8)
Au1—P1 (1)	2.2200 (8)	Au4—P4 (2)	2.2260 (9)
Angles, º			
P1—Au1—Cl1	178.38 (4)	P3B—Au3B—Cl3B	175.1 (4)
Cl2B—Au2B—P2	174.16 (5)	P3A—Au3A—Cl3A	172.9 (5)
P2—Au2A—Cl2A	172.57 (5)	P4—Au4—Cl4	176.25 (3)
Au2·1.8CH_2Cl_2			
Distances, Å			
Au1—Cl2	2.2775 (13)	P1—Au2	2.2423 (10)
Au2—Cl4	2.2813 (10)	Au1—P2	2.2357 (11)
Angles, º			
P2—Au1—Cl2	173.99 (5)	P1—Au2—Cl4	177.35 (4)

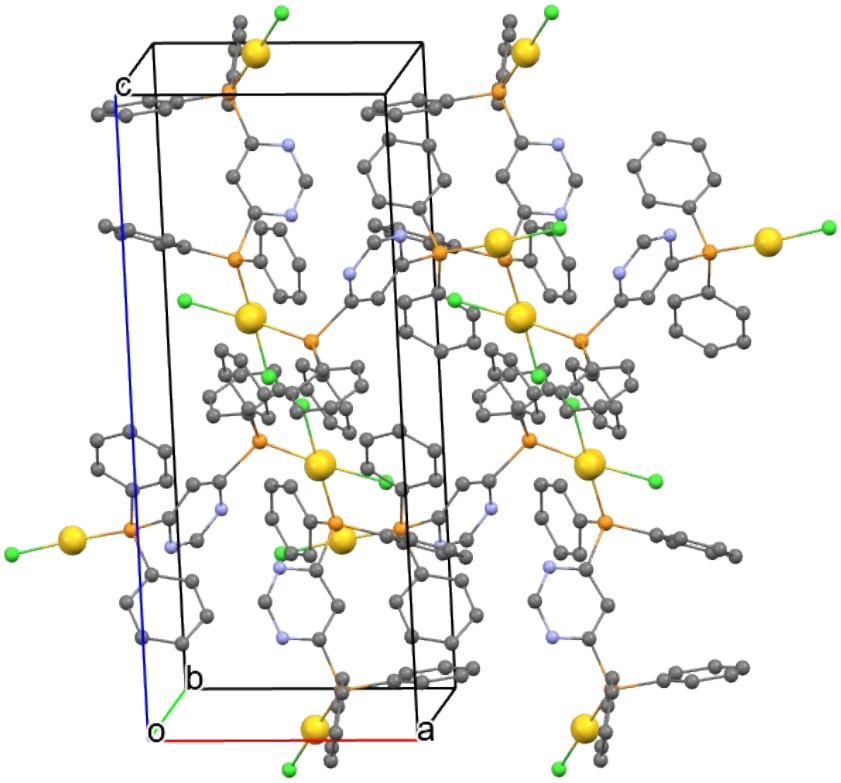

Fig. S1. Molecular packing of **Au1**

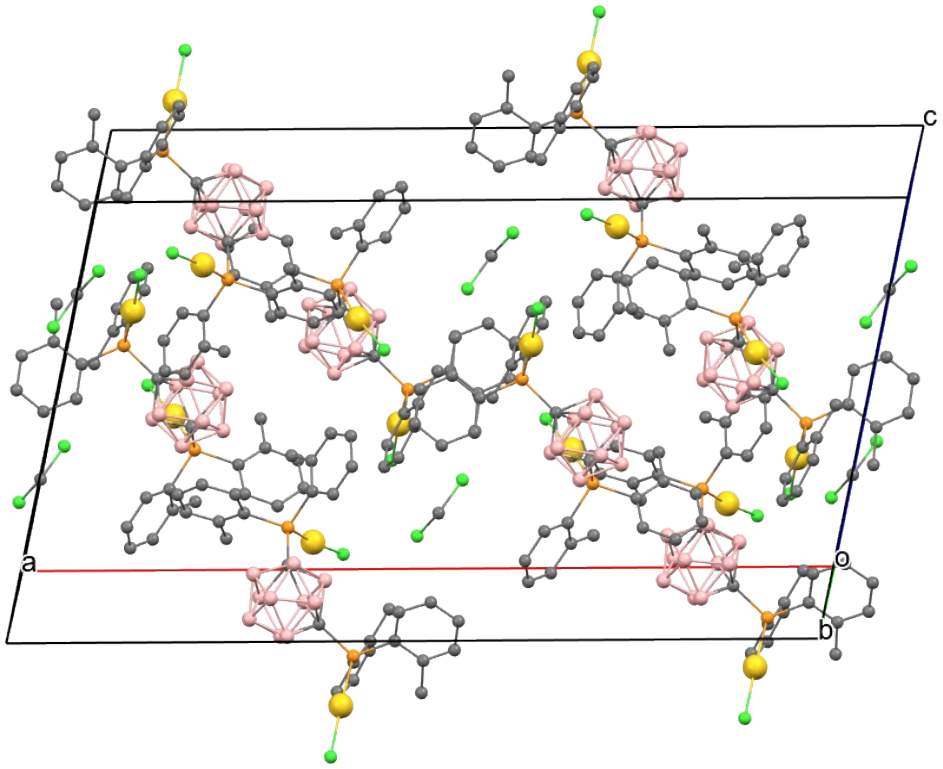

Fig. S2. Molecular packing of **Au2**·1.8CH_2Cl_2

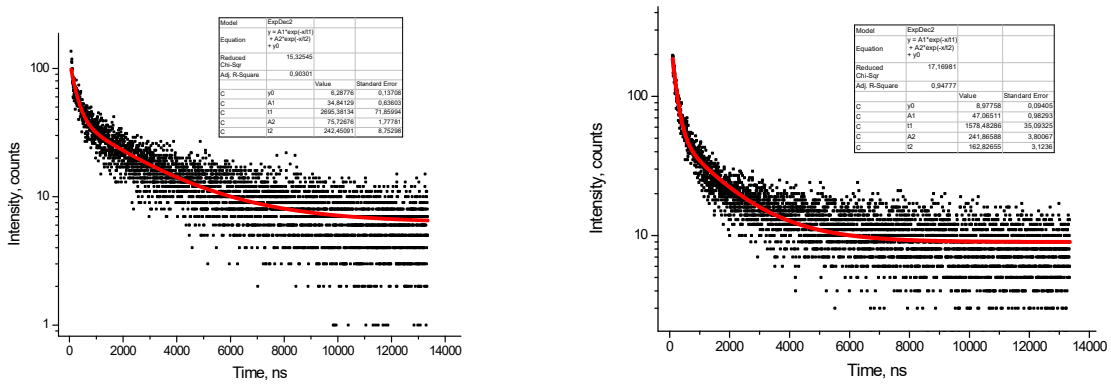

Fig. S3. Decay time for **Au1** (left) and **Au2** (right), T = 300 K

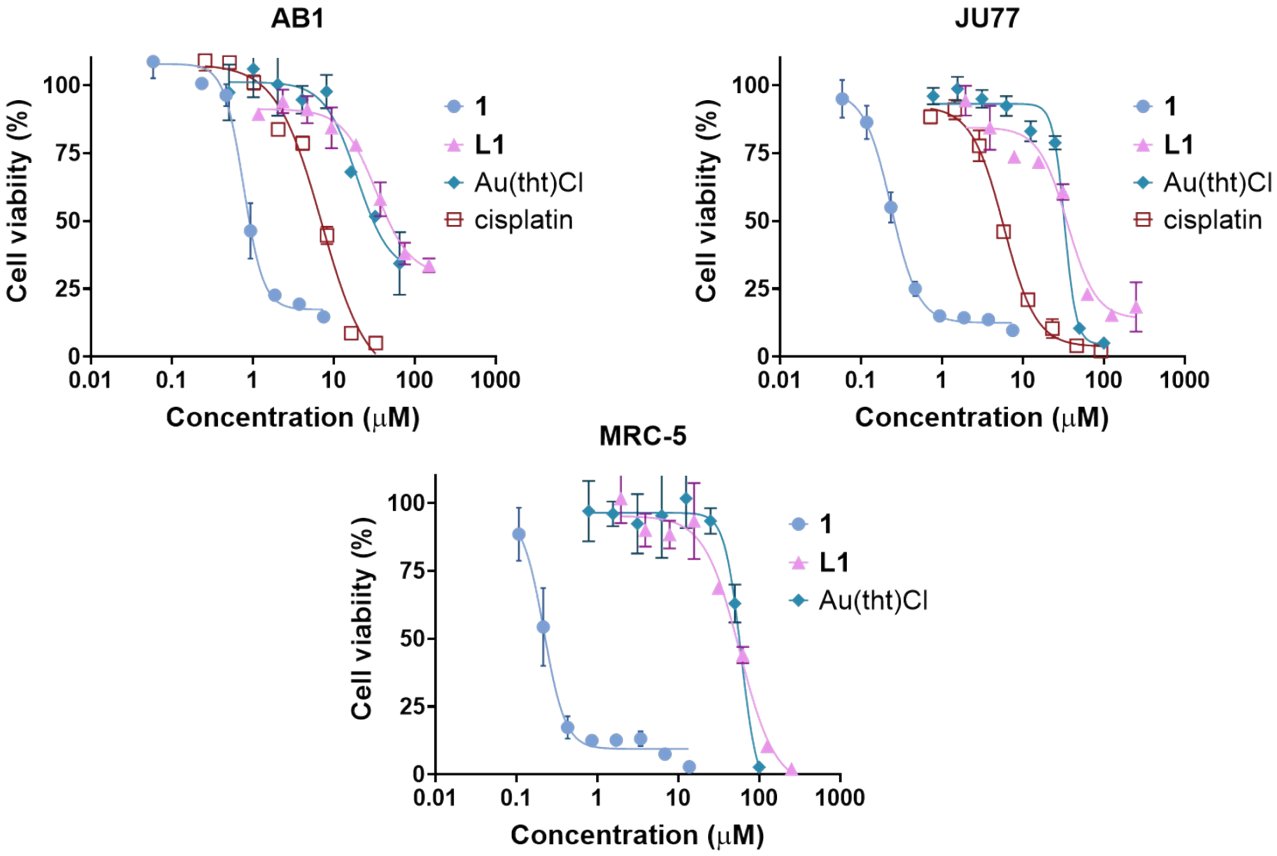

Fig. S4. Concentration-effect curves for **Au1**, L1, Au(tht)Cl, and cisplatin in AB1, JU77, and MRC-5 cell lines upon 72 h exposure

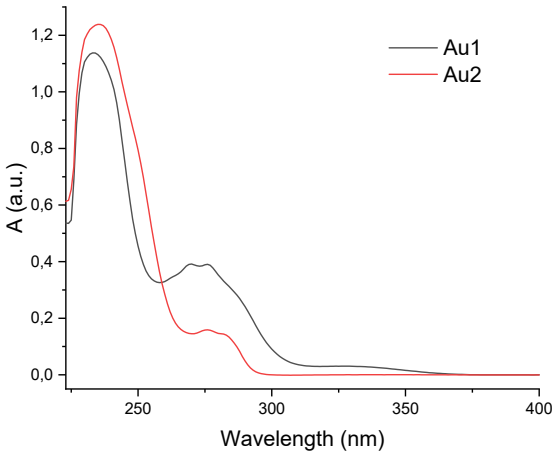

Fig. S5. UV-Vis spectra of complexes **Au1** and **Au2** in CH_2Cl_2