Electronic Supporting Information

Self-Assembly of Oxamidato Bridged Ester Functionalised Dirhenium Metallastirrups: Synthesis, Characterisation and Cytotoxicity Studies

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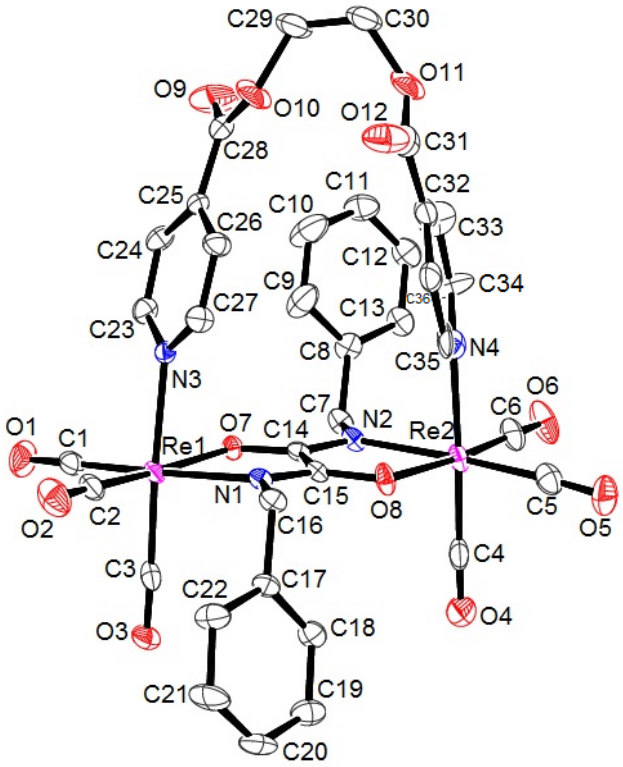

Fig. S1 ORTEP diagram of benzyloxamidato bridged dirhenium metallastirrup [$(CO)_3$Re(μ-dbno)(μ-etdp)Re$(CO)_3$] (**4**) with thermal ellipsoids at the 50% probability level.

Table S1 Selected bond lengths (Å) and angles (°) for **(4)**

Re1–N1	2.169(3)	O7–Re1–N1	75.86(10)
Re1–N3	2.219(3)	N1–Re1–N3	86.03(11)
Re1–O7	2.164(2)	N3–Re1–O7	78.85(10)
Re1–C1	1.907(4)	C2–Re1–N1	97.24(15)
Re1–C2	1.898(4)	C1–Re1–N3	92.42(14)
Re1–C3	1.929(4)	C3–Re1–N1	91.99(14)

Table S2 Crystallographic data and structure refinement details of compounds **2–5**

	2	**3**	**4**	**5**
empirical formula	$C_{42}H_{30}Cl_4N_4O_{12}Re_2$	$C_{68}H_{44}N_8O_{24}Re_4$	$C_{36}H_{26}N_4O_{12}Re_2$	$C_{36}H_{26}N_4O_{12}Re_2$
fw	1296.90	2101.91	1079.01	1079.01
cryst syst	orthorhombic	monoclinic	triclinic	monoclinic
space group	*Pccn*	*P*21/*n*	*P*-1	*P*21/*c*
temp (K)	120(10)	120(10)	121(2)	150(14)
a (Å)	11.2867(2)	18.7142(4)	10.8506(4)	12.0831(3)
b (Å)	14.1080(3)	17.8406(3)	13.0413(4)	10.9522(3)
c (Å)	29.1927(7)	22.0857(6)	14.1715(6)	27.2281(6)
α (°)	90.00	90.00	68.875(3)	90.00
β (°)	90.00	111.555(2)	71.963(4)	99.326(3)
γ (°)	90.00	90.00	88.975(3)	90.00
volume (Å^3)	4648.42(17)	6858.1(3)	1768.71(12)	3555.66(15)
Z	4	4	2	4
D_{calc} (mg mm^{-3})	1.853	2.036	2.026	2.016
μ (mm^{-1})	5.497	7.124	6.909	6.873
F (000)	2496.0	4000.0	1032.0	2064.0
crystal size (mm)	0.25 × 0.2 × 0.16	0.5 × 0.48 × 0.4	0.2 × 0.2 × 0.02	0.4 × 0.35 × 0.28
2θ range for data collection (deg)	7.22 to 58.44	7.14 to 58.32	7.42 to 58.3	7.44 to 50
reflns collected/unique	24145/5647	36753 /15854	19179/ 8155	19342/ 6232
R_{int}	0.0299	0.0390	0.0320	0.0304
data/restraints/params	5647/2/277	15854/0/937	8155/504/551	6232/165/488
goodness-of-fit on F^2	1.115	1.064	1.025	1.124
final *R* indices [I ≥ 2σ (I)]	R_1 = 0.0602 wR_2 = 0.1592	R_1 = 0.0373 wR_2 = 0.0937	R_1 = 0.0272 wR_2 = 0.0514	R_1 = 0.0293 wR_2 = 0.0570
final *R* indices [all data]	R_1 = 0.0737 wR_2 = 0.1669	R_1 = 0.0435 wR_2 = 0.0987	R_1 = 0.0410 wR_2 = 0.0554	R_1 = 0.0411 wR_2 = 0.0612
largest diff. peak and hole (e Å^{-3})	4.78 and –4.55	2.42 and –2.24	0.87 and –1.13	0.96 and –1.61
CCDC number	1054799	1054800	1054801	1054802

Cytotoxicity assay

Cancer cells were seeded at a density of 1×10^6 cells per well in 96-well plates for 24 h, in 200 µL of DMEM supplemented with 10% fetal bovine serum. In order to evaluate the cytotoxic effect of the compounds on normal cells, human peripheral blood mononuclear cells (PBMCs) were isolated. Isolated PBMCs were suspended in RPMI media and cells at the density of 1×10^6 cells per well were seeded in 96-well plates and incubated overnight. Different concentrations (10 to 100 µM) of compounds and cisplatin (a positive control) dissolved in DMSO were treated in triplicates and incubated for 48 h at 37 °C in 5% CO_2 incubator. After the treatment, cells were incubated with MTT (10 µL; 5 mg/mL) at 37 °C for 3 h and formazan crystal formed was dissolved in 80 µL of DMSO. The plates were read at 590 nm on a scanning multiwell spectrophotometer. The IC_{50} values (concentration of the compounds to inhibit 50% of cells) were calculated using Graph pad prism 6.0 software. Data are represented as the average and standard deviation of two independent assays. The statistical significance of the data was analyzed by ANNOVA with the level of significance at $p < 0.05$.

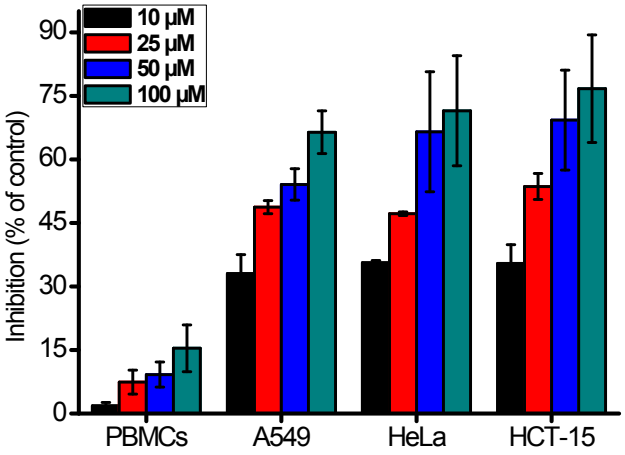

Fig. S2 Cytotoxicity activity of compound **1** at various concentrations (10, 25, 50 and 100 µM) in normal (PBMCs) and cancer (lung-A549, cervical-HeLa and colon-HCT-15) cells showing the dose-dependent inhibition of cancer cells based on MTT assay upon 48 h of exposure.

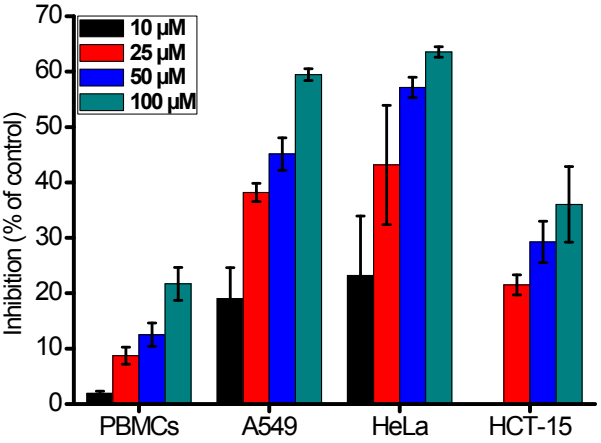

Fig. S3 Cytotoxicity activity of compound **2** at various concentrations (10, 25, 50 and 100 µM) in normal (PBMCs) and cancer (lung-A549, cervical-HeLa and colon-HCT-15) cells showing the dose-dependent inhibition of cancer cells based on MTT assay upon 48 h of exposure.

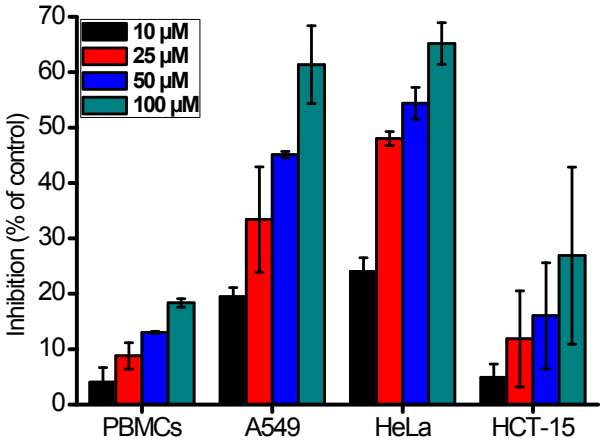

Fig. S4 Cytotoxicity activity of compound **3** at various concentrations (10, 25, 50 and 100 µM) in normal (PBMCs) and cancer (lung-A549, cervical-HeLa and colon-HCT-15) cells showing the dose-dependent inhibition of cancer cells based on MTT assay upon 48 h of exposure.

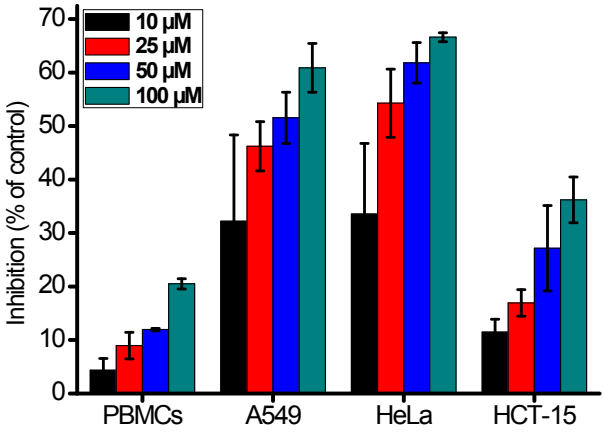

Fig. S5 Cytotoxicity activity of compound **4** at various concentrations (10, 25, 50 and 100 µM) in normal (PBMCs) and cancer (lung-A549, cervical-HeLa and colon-HCT-15) cells showing the dose-dependent inhibition of cancer cells based on MTT assay upon 48 h of exposure.

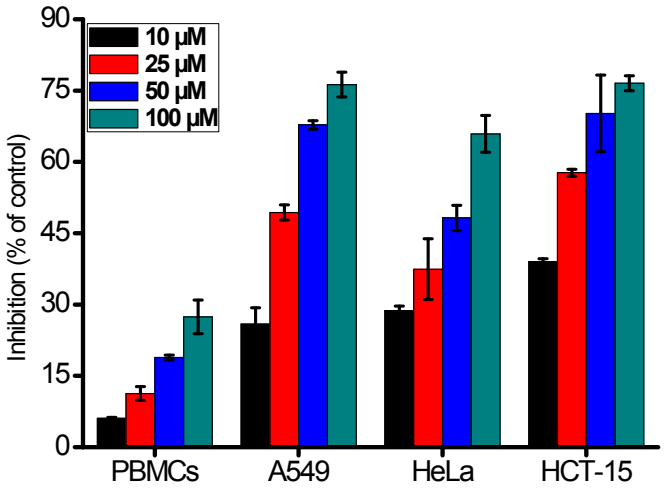

Fig. S6 Cytotoxicity activity of compound **5** at various concentrations (10, 25, 50 and 100 µM) in normal (PBMCs) and cancer (lung-A549, cervical-HeLa and colon-HCT-15) cells showing the dose-dependent inhibition of cancer cells based on MTT assay upon 48 h of exposure.

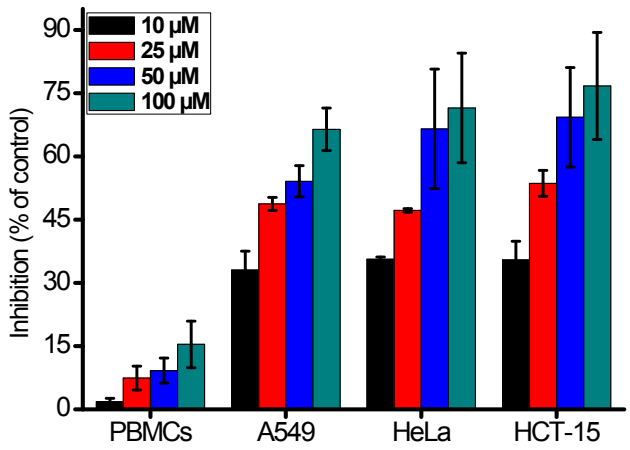

Fig. S7 Cytotoxicity activity of cisplatin at various concentrations (10, 25, 50 and 100 µM) in normal (PBMCs) and cancer (lung-A549, cervical-HeLa and colon-HCT-15) cells showing the dose-dependent inhibition of cancer cells based on MTT assay upon 48 h of exposure.