

# **Cytotoxicity, hydrophobicity, uptake and distribution of osmium(II) anticancer complexes in ovarian cancer cells**

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## **Supporting Information**

Spectroscopic data, ESI-MS and CHN analysis of complexes **1**, **2** and **4**.

Table S1

Figures S1-S6

### Spectroscopic data for the complexes

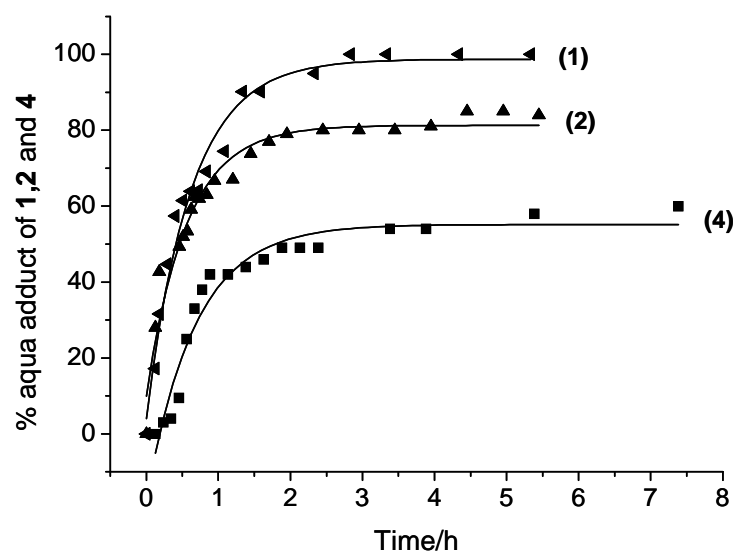
**[( $\eta^6$ -benzene)Os(4-methyl-picolinate)Cl] (1).** Anal. Calcd. for  $C_{13}H_{12}ClNO_2Os$  (439.92): C, 35.49; H, 2.75; N, 3.18%. Found: C, 35.08; H, 2.55; N, 3.27%. ESI-MS (+ve): 406.1  $m/z$ , [(bz)Os(4-Me-picolinate)]<sup>+</sup>. <sup>1</sup>H NMR (DMSO- $d_6$ ):  $\delta$  = 9.15 (1H, d,  $J$  = 5.52 Hz), 7.76 (1H, s), 7.5972 (d, 1H,  $J$  = 5.77 Hz), 6.20 (6H, s).

**[( $p$ -cymene)Os(4-methyl-picolinate)Cl] (2).** Anal. Calcd. for  $C_{17}H_{20}ClNO_2Os \cdot H_2O$  (514.04): C, 39.72; H, 4.31; N, 2.72%. Found: C, 38.97; H, 3.98; N, 2.90%. ESI-MS (+ve): 462.1  $m/z$ , [( $p$ -cym)Os(4-Me-picolinate)]<sup>+</sup>. <sup>1</sup>H NMR (MeOD- $d_4$ ):  $\delta$  = 8.96 (1H, d,  $J$  = 5.77 Hz), 7.87 (1H, s), 7.5728 (1H, dd,  $J$  = 5.52 and 1.51 Hz), 6.17 (2H, d,  $J$  = 5.52 Hz), 5.90 (2H, t,  $J$  = 6.02 Hz), 2.69 (1H, sept,  $J$  = 6.78 Hz), 2.61 (3H, s), 2.32 (3H, s), 1.23 (6H, dd,  $J$  = 7.03 and 11.04 Hz).

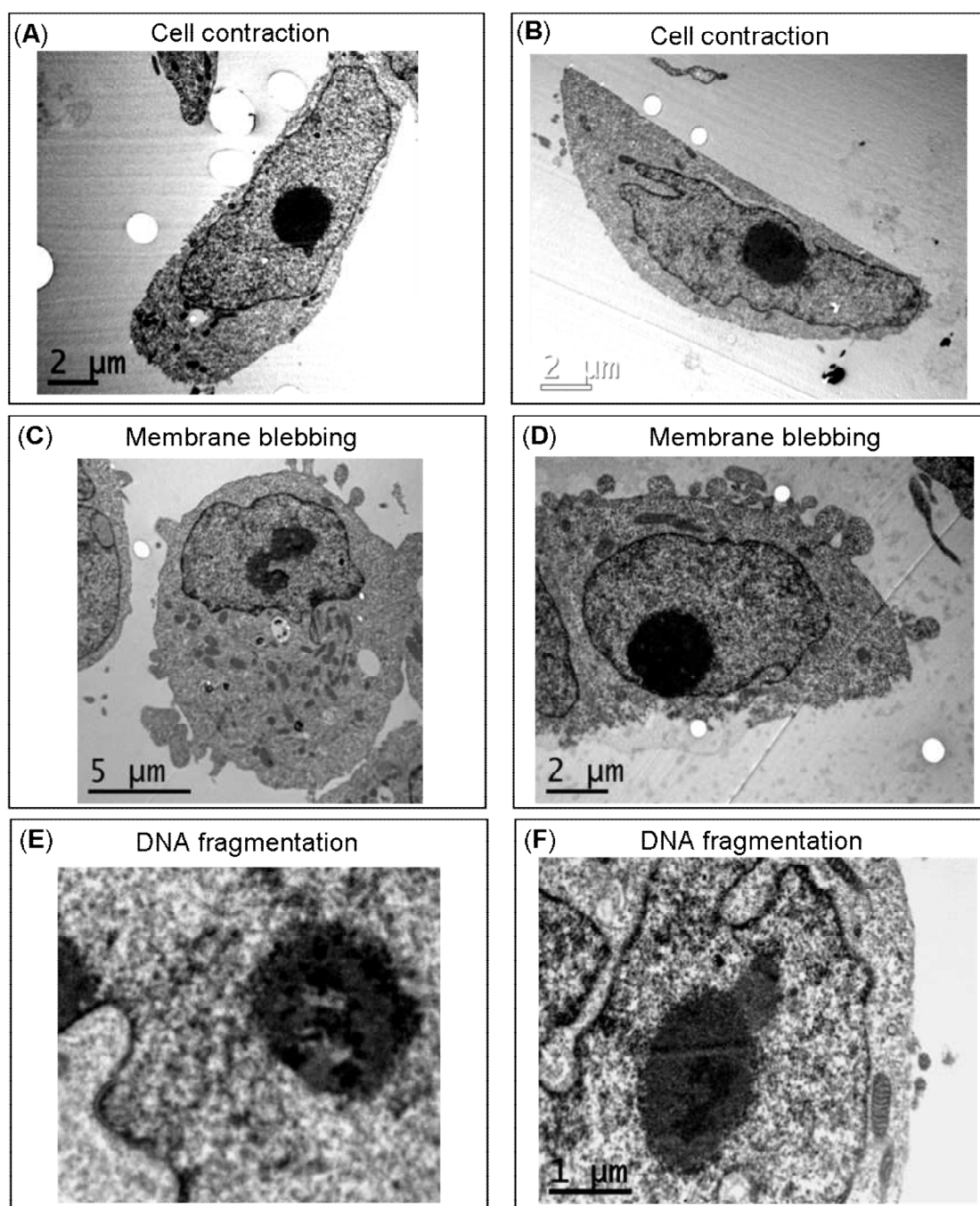
**[( $\eta^6$ -tetrahydroanthracene)Os(4-methyl-picolinate)Cl] (4).** Anal. Calcd. for  $C_{21}H_{18}ClNO_2Os$  (542.06): C, 46.53; H, 3.35; N, 2.58%. Found: C, 45.92; H, 3.18; N, 2.64%. ESI-MS (+ve): 510.1  $m/z$ , [(THA)Os(4-Me-picolinate)]<sup>+</sup>. <sup>1</sup>H NMR (DMSO- $d_6$ ):  $\delta$  = 9.03 (1H, d,  $J$  = 5.52 Hz), 7.71 (1H, s), 7.58 (1H, d,  $J$  = 4.77 Hz), 6.19 (1H, d,  $J$  = 5.27 Hz), 6.15 (1H, t,  $J$  = 5.02 Hz), 6.10 (1H, d,  $J$  = 5.52 Hz), 6.01 (1H, t,  $J$  = 5.02 Hz), 5.68 (2H, m), 5.64 (2H, m), 3.21 (1H, s), 3.05 (1H, m), 2.80 (2H, m), 2.71 (1H, s), 2.37 (1H, s), 2.12 (2H, m).

**Table S1.** Instrumental Settings for ICP-MS

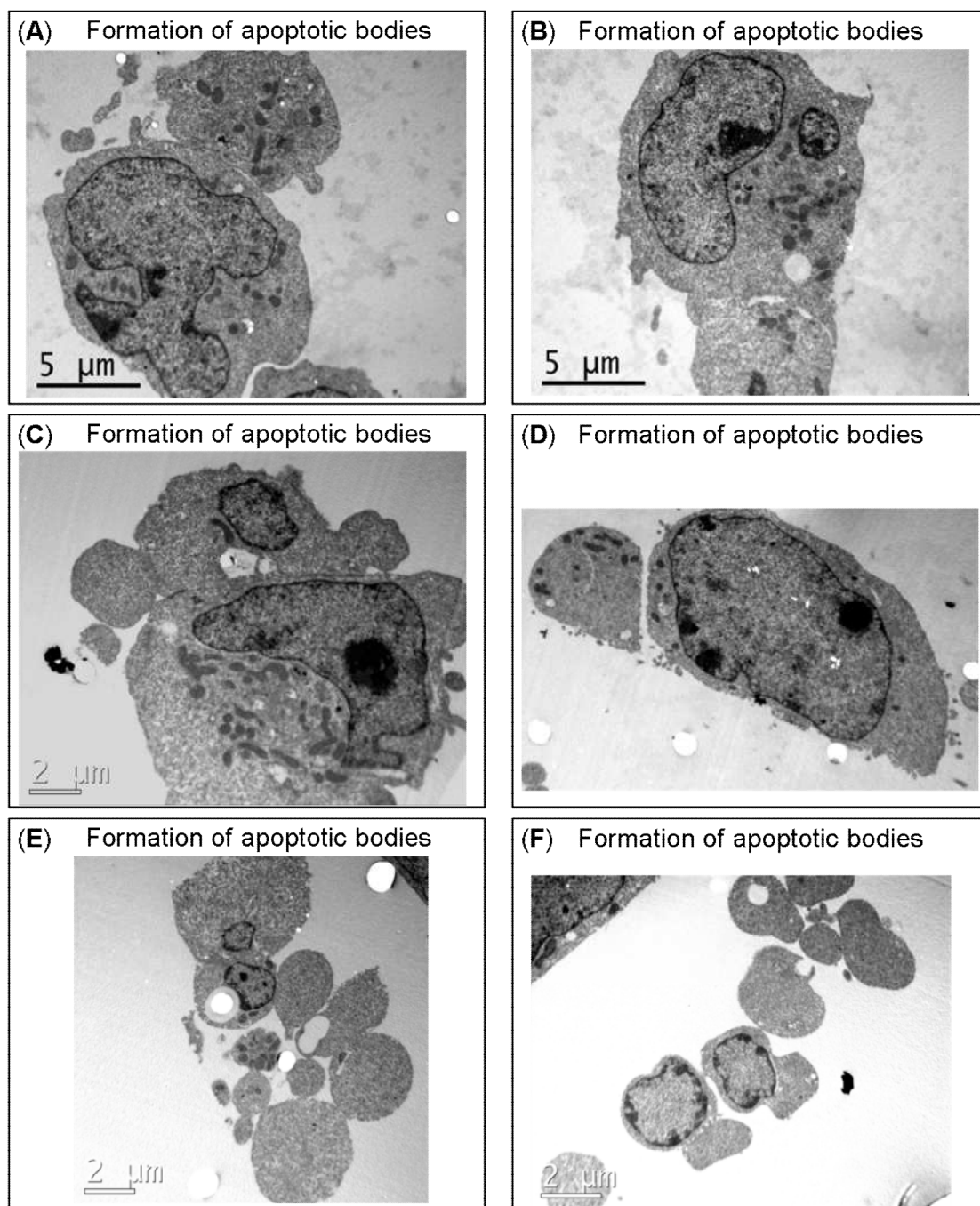
Plasma condition	
Plasma gas / Lmin <sup>-1</sup>	15
Auxiliary gas/ Lmin <sup>-1</sup>	0.2
Forward Power / W	1550
Reflected Power / W	1
RF Matching / V	1.8
Smpl Depth / mm	9
Carrier Gas / Lmin <sup>-1</sup>	0.9
Makeup Gas / Lmin <sup>-1</sup>	0.2
Nebulizer Pump / rps	0.08
S/C Temp/ degC	15
Analyser Pressure / Pa	10 <sup>-3</sup>
FF/BK Pressure / Pa	343
Peristaltic pump/ rpm	0.08
Ion Lenses	
Extract 1 / V	0
Extract 2 / V	-130
Omega Bias-ce / V	-16
Omega Lens-ce / V	1.8
Cell entrance / V	-20
QP focus / V	5
Cell Exit / V	-20
Q-pole Parameters	
AMU gain	127
AMU Offset	128
Axis gain	0.9998
Axis Offset	0
QP Bias/V	-5
Octopole Parameters	
OctP RF/ V	180
OctoP Bias/ V	-50
Detector Parameters	
Discriminator / mV	8
Analog HV / V	1730
Pulse HV / V	1070



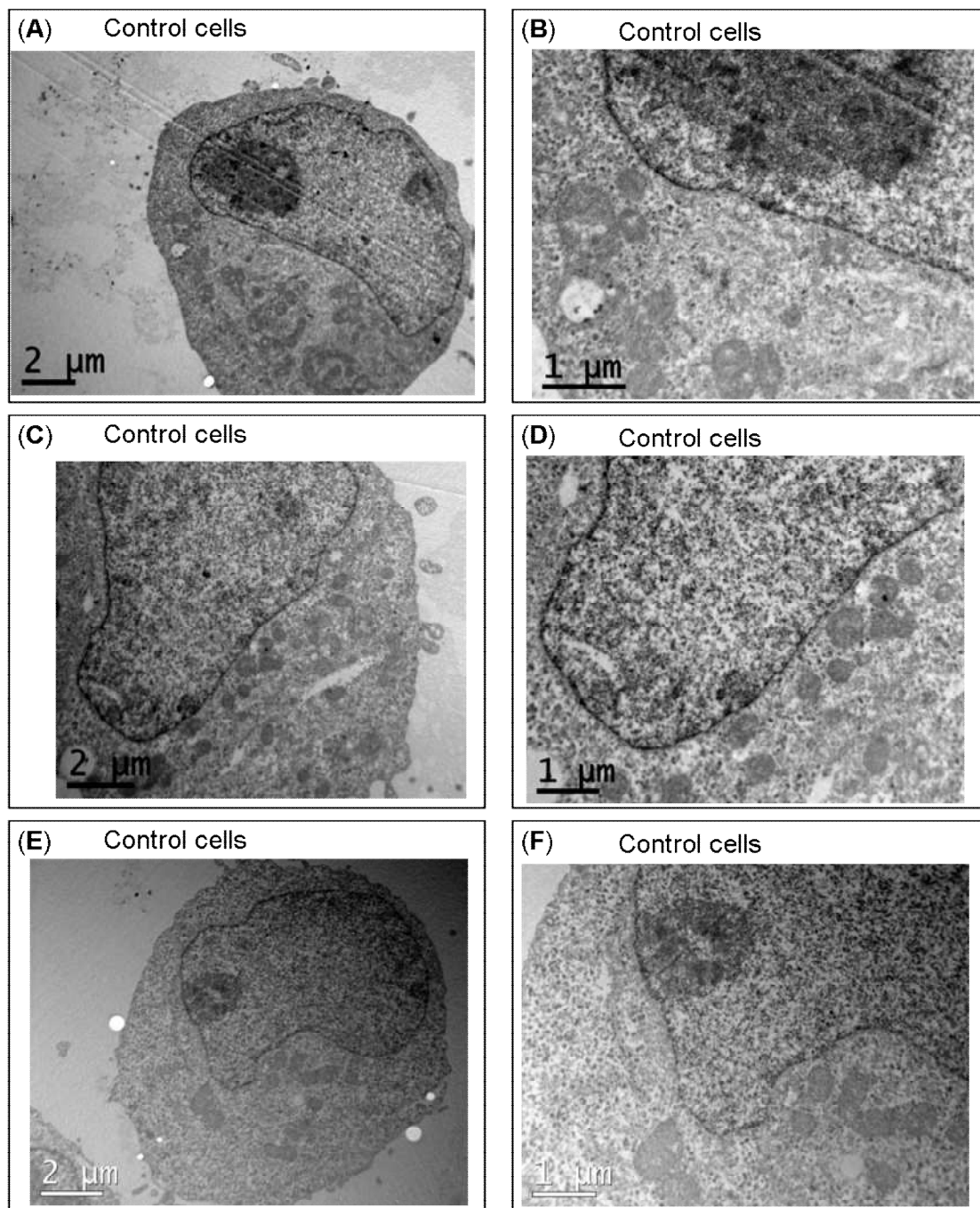
**Figure S1.** Time dependence for formation of the aqua complexes of **1**, **2** and **4** (based on  $^1\text{H}$  NMR peak integrals) during hydrolysis of **1**, **2** and **4** in acidic  $\text{D}_2\text{O}$  ( $\text{pH}^* 2$ ) at 288 K.



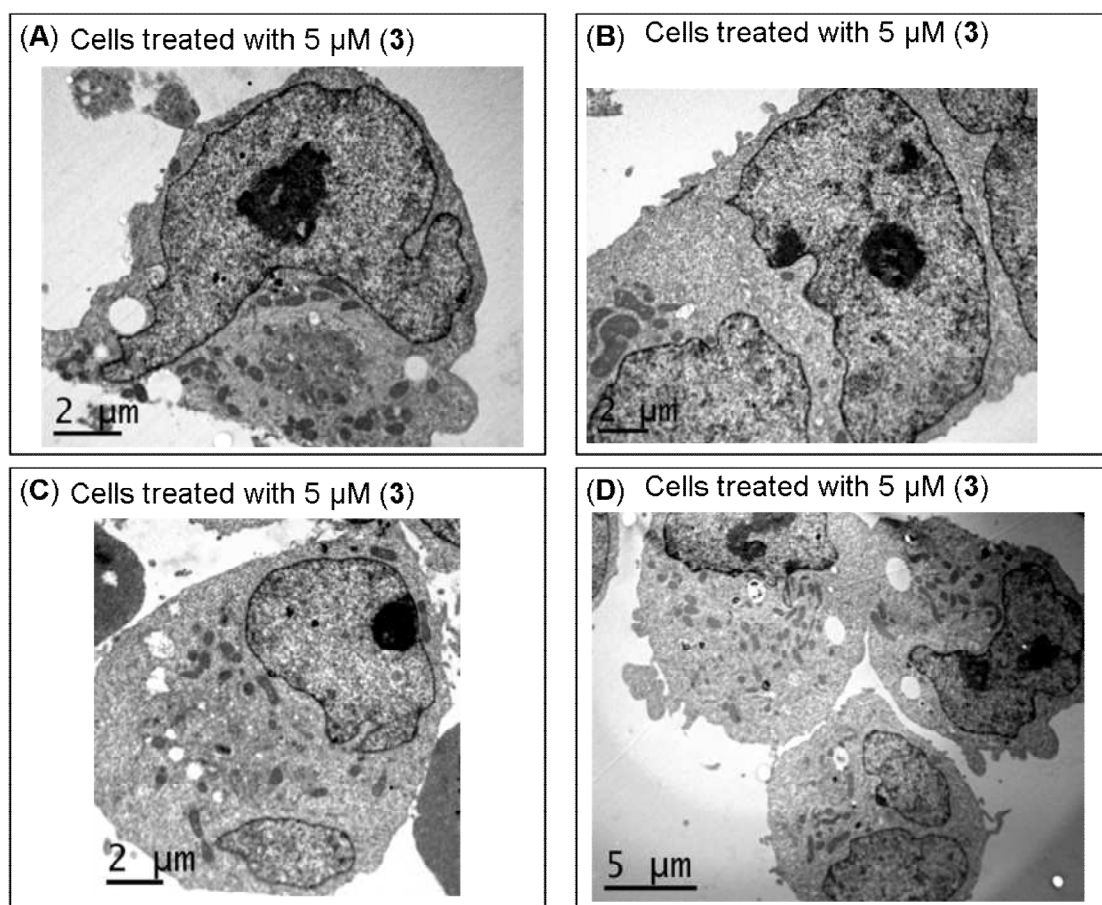
**Figure S2.** TEM images of A2780 cells exposed to complex **3**, showing the different stages of cell apoptosis; (A, B) cell contraction, (C, D) membrane blebbing, (E, F) DNA fragmentation.



**Figure S3.** (A-F) TEM images of A2780 cells exposed to complex **3**, showing the formation of apoptotic bodies, marking the final stage of cell apoptosis.

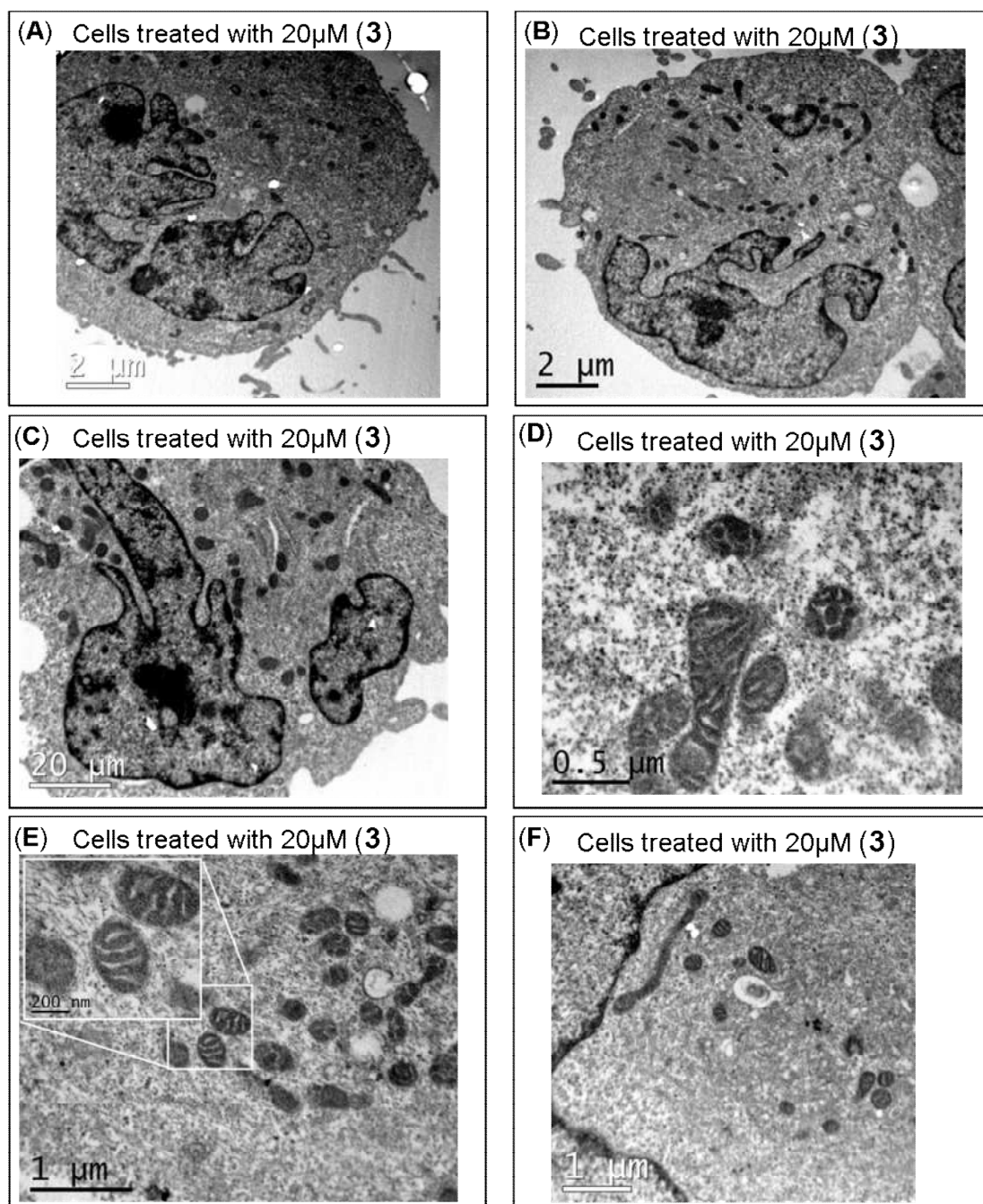


**Figure S4.** (A-F) TEM images of untreated A2780 cells (controls).



**Figure S5.** (A-D) TEM images of A2780 cells exposed to 5  $\mu$ M complex **3**.





**Figure S6.** (A-F) TEM images of A2780 cells exposed to 20  $\mu$ M complex **3**.