# **Supplementary information**

## 1. Spectroscopy of Complexes:

1.1. 1



Figure 1.1.1. <sup>1</sup>H-NMR of **1** in a mixture of deuterated water:acetonitrile (1:1).



Figure 1.1.2. UV/Vis and Emission spectra of 1 (25  $\mu$ M) in dichloromethane.  $\lambda_{exc}$ =425nm.







Figure 1.2.2. 2D-COSY <sup>1</sup>H-NMR of 2 in a mixture of deuterated water:acetonitrile (1:1).



Figure 3.10. UV/Vis and Emission spectra of 2 (25  $\mu$ M) in dichloromethane.  $\lambda_{exc}$ =425nm.



Figure 1.3.1. <sup>1</sup>H-NMR of **3** in a mixture of deuterated water:acetonitrile (1:1).



Figure 1.3.2. 2D-COSY <sup>1</sup>H-NMR of **3** in a mixture of deuterated water:acetonitrile (1:1).



Figure 1.3.3. UV/Vis and Emission spectra of **3** (25  $\mu$ M) in dichloromethane.  $\lambda_{exc}$ =480nm..





Figure 1.4.1. <sup>1</sup>H-NMR of **4** in a mixture of deuterated water:acetonitrile (1:1).



Figure 1.4.2. UV/Vis and Emission spectra of  $\boldsymbol{4}$  (25  $\mu M)$  in dichloromethane.  $\lambda_{exc}{=}480nm.$ 





Figure 1.5.1. <sup>1</sup>H-NMR of **5** in a mixture of deuterated water:acetonitrile (1:1).



Figure 1.5.2. UV/Vis and Emission spectra of 5 (25  $\mu$ M) in dichloromethane.  $\lambda_{exc}$ =480nm...

### 2. Cytotoxicity

Molecule	T-47D	MDA-MB-231	SK-OV-3	A2780	A2780cisR	Rx <sup>[a]</sup>
1	$15.4 \pm 0.1$	6.3 ± 1	19.3 ± 1.2	$2.6\pm0.7$	$5.9\pm0.9$	2.2
2	12.3 ± 1.9	11.4 ± 1.2	$19.8\pm2.6$	$4.3\pm0.9$	11.8 ± 1.8	2.8
3	2.1 ± 1.5	4± 1.4	$15.5 \pm 0.4$			
4	52.2 ± 2.6	50.1± 5.9	83.8 ± 4.2			
5	22.2 ± 2.9	30.5± 7.8	39.4 ± 9.1			
Cisplatin	28 ± 3	31.3 ± 4.7	$11.2 \pm 0.1$	$3.0 \pm 0.5$	12.8 ± 1.4	4.3

Table 2.1. IC  $_{50}$  µM of synthesised complexes against Breast and ovarian cancer cell lines.

[a] Rx is ratio of IC50 for a compound in A2780cisR compared to A2780. \* indicate a oestradiol derivative.

#### 3. Cellular uptake

	SK-OV-3			T-47D			MDA-MB-231		
	whole cell	cytoplasm	nuclei	whole cell	cytoplasm	nuclei	whole cell	cytoplasm	nuclei
1	$159\pm14$	111 ± 11	$41\pm 5$	130	$80\pm19$	$30\pm 1$	$361\pm23$	61 ± 13	$33\pm14$
2	<b>474</b> ± 7	<b>97</b> ± 8	<b>28</b> ± 2	$408\pm26$	<b>53</b> ± 12	<b>17</b> ± 1	<b>287</b> ± 11	<b>67</b> ± 5	<b>26</b> ± 1
3	749	<b>137</b> ± 7	129	<b>204</b> ± 21	77	$101\pm0.3$	<b>630</b> ± 53	<b>160</b> ± 6	<b>160</b> ± 11
Cisplatin	$25 \pm 12$	$12\pm 2$	$1.4 \pm 0.4$	11 ± 2	5	0.2	$9\pm0.1$	8 ± 1.6	$2\pm0.1$

Table 3.1 pmoles of Pt in T-47D, SK-OV-3 and MDA-MB-231 per million cells after 3 hours of treatment with  $30 \mu M$  of complexes.



## 4. Stability of complexes

Figure 4.1. UV/Vis of **1** (left) and **2** (right) (50 µM) during 72h in water (top), RPMI 1640 (middle) and DMEM medium (bottom).





Figure 5.1. Displacement of ethidium bromide (15 μM) from ct-DNA (12 μM) by sinthesized complexes. Mixing ratios EB/complex are shown in the caption. λexc=480nm. Decreasing ratios of emission (bottom right).



Figure 5.2. Effect on free ethidium bromide (15  $\mu$ M) fluorescence by sinthesized complexes. Mixing ratios EB/complex are shown in the caption.  $\lambda$ exc=480nm. Decreasing ratios of emission (bottom right).



#### 6 Circular and linear Dichroism

Figure 6.1. CD absorbance of the complexes at equivalent concentration to the 5-1 (DNA(bp):complex) titration point (A); ct-DNA titration with 5 (B); ct-DNA titration with 5 after subtraction of the CD absorbance of the free complex (C); CD absorbance spectrum and ICD signal at the 5-1 DNA(bp):complex point.



Table 6.2. CD spectra of titration of ct-DNA(300 μM in 20 mM NaCl and 0.89 mM Sodium Cacodylate pH 6.8) with **1**, **2**, **3** (third), **4** and **5**. Corrected substracting CD absorbance of the complexes.

#### 7 DNA Fluorescence tritation



Figure 7.1. Fluorescence response of the complexes observed on addition of DNA (bp): normalized to maximum of fluorescence observed (A); related to maximum of fluorescence of the complexes at 25  $\mu$ M in dichloromethane (B).