Electronic Supplementary Material (ESI) for Dalton Transactions.

Supporting information

Catalytic transfer hydrogenation and anticancer activity of arene-ruthenium compounds incorporating bi-dentate precursors

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Contents

Table S1. SRB assay results for PC-3 and DU145 cells

Compound	Molecular weight	SRB assay (GI_{50}, μM) N=3	
		PC-3 cells	DU145 cells
2	416.86	>100	>100
3	421.97	16.6±2.7	6.4±0.8
4	469.00	7.7±0.8	6.7±0.4
7	521.12	14.9±2.6	10.3±1.4
Cisplatin	300.05	27.0±6.1	22.8±5.1

Table S2. Hydrogen bonds for **2** [Å and °].

D-H...A	d(D-H)	d(H...A)	d(D...A)	<(DHA)
O(7)-H(7B)...O(6)#1	0.82	1.78	2.598(16)	178.5
O(8)-H(8B)...O(6)#1	0.82	2.27	3.018(17)	151.2
N(2)-H(2A)...O(2)#2	0.89	2.11	2.938(14)	153.9
N(2)-H(2B)...O(1)#2	0.89	2.64	3.088(15)	112.2
O(4)-H(4B)...O(2)#3	0.82	1.74	2.562(15)	178.0
N(1)-H(1A)...O(5)	0.89	2.38	3.103(15)	138.5
N(1)-H(1E)...O(6)	0.89	2.38	2.997(15)	126.2
N(2)-H(2B)...Cl(2)	0.89	2.68	2.996(12)	102.4

Symmetry transformations used to generate equivalent atoms:
#1 -x,y+1/2,-z+1/2 #2 x,y+1,z #3 -x+1,y+1/2,-z+1/2

Figure S1. Effect of compound **4** on the expression of several proteins. PC-3 cells were incubated in the absence or presence of compound 4 (20 µM) for the indicated times. The cells were harvested and lysed for the detection of the indicated protein expression by Western blot analysis. The expression was quantified using the computerized image analysis system ImageQuant (Amersham Biosciences). The data are expressed as mean±SEM of three to four independent experiments. * *P*< 0.05,** *P*< 0.01 and *** *P*< 0.001 compared with 100% control.

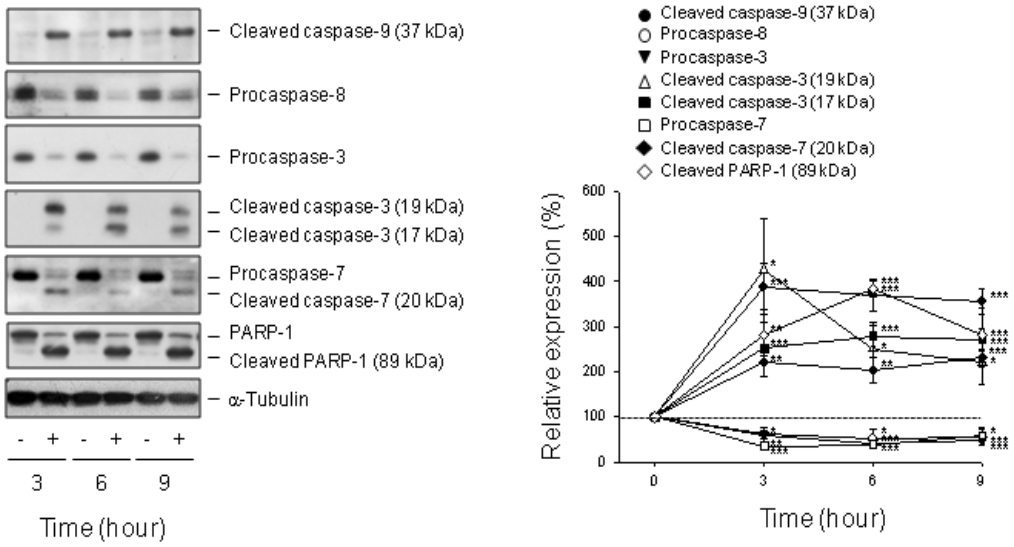
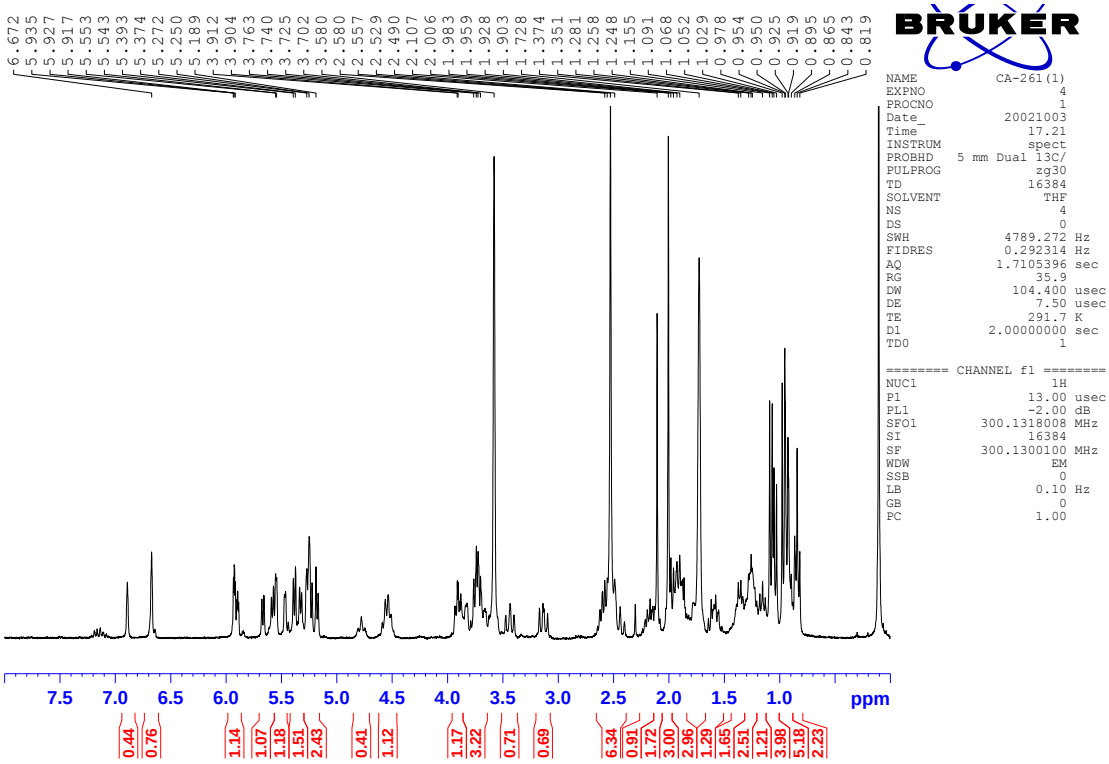


Figure S2. ^{1}H NMR spectrum of compound **7** in d^{8}-THF using a 300 MHz NMR spectrometer



Western blotting (experimental). After the treatment, cells were harvested with trypsinization, centrifuged and lysed in 0.1 ml of lysis buffer containing 10 mMTris-HCl (pH 7.4), 150 mMNaCl, 1mM EGTA, 1 % Triton X-100, 1 mM PMSF, 10 μg/ml leupeptin, 10 μg/ml aprotinin, 50 mMNaF and 100 μM sodium orthovanadate. Total protein was quantified, mixed with sample buffer and boiled at 90^{o}C for 5 min. Equal amount of protein (30 μg) was separated by electrophoresis in 8 or 12 % SDS-PAGE, transferred to PVDF membranes and detected with specific antibodies. The immune-reactive proteins after incubation with appropriately labeled secondary antibody were detected with an enhanced chemiluminescence detection kit (Amersham, Buckinghamshire, UK).

Data analysis (experimental). Data are presented as the mean±SEM for the indicated number of separate experiments. Statistical analysis of data for multiple groups is performed with one-way analysis of variance. Student's *t*-test is applied for comparison of two groups. *P*-values less than 0.05 are statistically considered significant.