Electronic Supplementary Material (ESI) for Dalton Transactions.

Supplementary Information

The Contrasting Catalytic Efficiency and Cancer Cell Antiproliferative Activity of Stereoselective Organoruthenium Transfer Hydrogenation Catalysts

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Tables S1 – S5

Figures S1 – S9

Table S1. Anticancer activity in the NCI 60-cell line screen, measured as the GI_{50}. (A) complex **8**, (B) complex **8a**.

(A) Complex **8.**

National Cancer Institute Developmental Therapeutics Program
In-Vitro Testing Results

NSC : D - 756775 / 1	Experiment ID : 1105NS53	Test Type : 08	Units : Molar
Report Date : July 15, 2011	Test Date : May 23, 2011	QNS :	MC :
COMI : MW02 (103477)	Stain Reagent : SRB Dual-Pass Related	SSPL : 0Y4T	

			Log10 Concentration											
	Time	Mean Optical Densities						Percent Growth						
Panel/Cell Line	Zero	Ctrl	-8.0	-7.0	-6.0	-5.0	-4.0	-8.0	-7.0	-6.0	-5.0	-4.0	GI50	TGI	LC50
Leukemia															
CCRF-CEM	0.527	1.752	1.825	.	1.079	0.277	0.336	106	.	45	-48	-36	6.88E-7	3.07E-6	> 1.00E-4
HL-60(TB)	0.594	2.626	2.259	.	1.753	0.346	0.286	82	.	57	-42	-52	1.18E-6	3.77E-6	6.43E-5
K-562	0.249	1.922	1.861	.	0.725	0.162	0.154	96	.	28	-35	-38	2.32E-7	2.81E-6	> 1.00E-4
MOLT-4	0.587	2.273	2.220	.	2.008	0.446	0.563	97	.	84	-24	-4	2.07E-6	5.99E-6	> 1.00E-4
RPMI-8226	0.789	2.570	2.511	.	1.807	0.470	0.505	97	.	57	-40	-36	1.18E-6	3.85E-6	> 1.00E-4
SR	0.346	1.724	1.654	.	1.248	0.272	0.288	95	.	65	-21	-17	1.51E-6	5.67E-6	> 1.00E-4
Non-Small Cell Lung Cancer															
A549/ATCC	0.315	1.517	1.469	.	1.384	0.441	0.079	96	.	89	10	-75	3.14E-6	1.33E-5	5.11E-5
EKVX	0.746	1.683	1.620	.	1.570	0.211	0.048	93	.	88	-72	-94	1.73E-6	3.55E-6	7.30E-6
HOP-62	0.348	0.971	0.954	.	0.987	0.104	0.080	97	.	102	-70	-77	2.01E-6	3.92E-6	7.63E-6
NCI-H226	0.605	1.673	1.587	.	1.469	0.147	0.245	92	.	81	-76	-60	1.57E-6	3.28E-6	6.85E-6
NCI-H23	0.538	1.438	1.390	.	1.339	0.079	0.218	95	.	89	-85	-60	1.67E-6	3.24E-6	6.27E-6
NCI-H322M	0.821	1.687	1.652	.	1.739	1.347	0.036	96	.	106	61	-96	1.17E-5	2.45E-5	5.11E-5
NCI-H460	0.226	1.792	1.785	.	1.682	0.113	0.146	100	.	93	-50	-35	2.00E-6	4.47E-6	> 1.00E-4
NCI-H522	0.593	1.547	1.463	.	1.065	0.052	0.086	91	.	50	-91	-85	9.46E-7	2.25E-6	5.09E-6
Colon Cancer															
COLO 205	0.270	1.306	1.358	.	1.098	0.080	0.163	105	.	80	-71	-40	1.58E-6	3.40E-6	.
HCC-2998	0.685	2.008	2.086	.	1.990	0.062	0.048	106	.	99	-91	-93	1.81E-6	3.31E-6	6.08E-6
HCT-116	0.186	1.124	1.136	.	0.681	0.023	0.036	101	.	53	-88	-81	1.05E-6	2.38E-6	5.40E-6
HCT-15	0.472	2.547	2.414	.	2.335	0.210	0.100	94	.	90	-56	-79	1.88E-6	4.15E-6	9.16E-6
HT29	0.217	1.055	1.084	.	1.053	0.066	0.085	103	.	100	-70	-61	1.96E-6	3.87E-6	7.64E-6
KM12	0.439	1.948	1.847	.	1.928	0.456	0.053	93	.	99	1	-88	3.16E-6	1.03E-5	3.74E-5
SW-620	0.228	1.313	1.292	.	0.645	0.041	0.072	98	.	38	-82	-69	4.09E-7	2.08E-6	5.40E-6
CNS Cancer															
SF-268	0.469	1.537	1.499	.	1.496	0.068	0.052	96	.	96	-86	-89	1.79E-6	3.38E-6	6.37E-6
SF-295	0.640	1.977	1.887	.	1.863	0.882	0.123	93	.	91	18	-81	3.68E-6	1.52E-5	4.88E-5
SF-539	0.834	2.105	2.002	.	2.053	0.109	0.346	92	.	96	-87	-59	1.78E-6	3.34E-6	6.28E-6
SNB-19	0.448	1.318	1.278	.	1.306	0.254	0.061	95	.	99	-43	-86	2.20E-6	4.95E-6	1.43E-5
SNB-75	0.603	1.275	1.284	.	1.229	0.058	0.398	101	.	93	-90	-34	1.72E-6	3.22E-6	.
U251	0.254	1.187	1.153	.	0.723	0.006	0.031	96	.	50	-98	-88	1.00E-6	2.19E-6	4.76E-6
Melanoma															
LOX IMVI	0.221	1.342	1.322	.	1.108	0.013	0.060	98	.	79	-94	-73	1.47E-6	2.86E-6	5.55E-6
MALME-3M	0.694	1.411	1.419	.	1.207	0.180	0.343	101	.	72	-74	-51	1.41E-6	3.10E-6	6.83E-6
M14	0.393	1.239	1.199	.	1.156	0.029	0.032	95	.	90	-93	-92	1.66E-6	3.11E-6	5.84E-6
MDA-MB-435	0.445	1.943	1.906	.	1.767	0.069	0.135	97	.	88	-84	-70	1.66E-6	3.24E-6	6.31E-6
SK-MEL-2	0.990	1.689	1.676	.	1.660	0.195	0.245	98	.	96	-80	-75	1.82E-6	3.50E-6	6.73E-6
SK-MEL-28	0.516	1.451	1.478	.	1.433	0.067	0.224	103	.	98	-87	-57	1.82E-6	3.39E-6	6.31E-6
SK-MEL-5	0.442	2.658	2.673	.	2.573	0.610	0.025	101	.	96	8	-94	3.32E-6	1.19E-5	3.67E-5
UACC-257	0.776	1.473	1.418	.	1.351	0.058	0.138	92	.	83	-93	-82	1.53E-6	2.96E-6	5.71E-6
UACC-62	0.834	2.246	2.199	.	2.097	0.075	0.108	97	.	89	-91	-87	1.65E-6	3.13E-6	5.93E-6
Ovarian Cancer															
IGROV1	0.523	1.661	1.683	.	1.667	0.166	0.419	102	.	101	-68	-20	1.99E-6	3.94E-6	.
OVCAR-3	0.499	1.316	1.316	.	1.235	0.014	0.020	100	.	90	-97	-96	1.64E-6	3.02E-6	5.59E-6
OVCAR-4	0.488	1.523	1.462	.	1.301	0.210	0.412	94	.	79	-57	-16	1.62E-6	3.79E-6	.
OVCAR-5	0.573	1.498	1.446	.	1.462	0.235	0.117	94	.	96	-59	-80	1.98E-6	4.16E-6	8.74E-6
OVCAR-8	0.386	1.480	1.506	.	1.228	0.077	0.337	102	.	77	-80	-13	1.48E-6	3.09E-6	.
NCI/ADR-RES	0.452	1.295	1.310	.	1.270	0.707	0.331	102	.	97	30	-27	5.06E-6	3.39E-5	> 1.00E-4
SK-OV-3	0.503	1.316	1.297	.	1.349	0.758	0.024	98	.	104	31	-95	5.54E-6	1.77E-5	4.39E-5
Renal Cancer															
786-0	0.533	1.814	1.731	.	1.852	0.061	0.023	94	.	103	-89	-96	1.89E-6	3.45E-6	6.28E-6
A498	1.239	2.180	2.087	.	2.144	1.723	0.018	90	.	96	51	-99	1.02E-5	2.20E-5	4.74E-5
ACHN	0.418	1.439	1.400	.	1.200	0.015	0.009	96	.	77	-96	-98	1.42E-6	2.77E-6	5.39E-6
CAKI-1	0.688	2.077	2.104	.	2.020	0.305	0.383	102	.	96	-56	-44	2.01E-6	4.29E-6	.
RXF 393	0.541	1.151	1.155	.	1.041	0.016	-0.004	101	.	82	-97	-100	1.51E-6	2.87E-6	5.46E-6
SN12C	0.583	1.777	1.729	.	1.642	0.123	0.315	96	.	89	-79	-46	1.70E-6	3.38E-6	.
TK-10	0.657	1.128	1.084	.	1.074	0.023	0.012	91	.	89	-96	-98	1.62E-6	3.01E-6	5.61E-6
UO-31	0.566	1.699	1.582	.	1.599	0.014	0.042	90	.	91	-98	-93	1.65E-6	3.04E-6	5.60E-6
Prostate Cancer															
PC-3	0.488	1.113	1.095	.	1.055	0.075	0.133	97	.	91	-85	-73	1.71E-6	3.29E-6	6.34E-6
DU-145	0.300	1.099	1.071	.	0.404	0.009	0.009	97	.	13	-97	-97	1.30E-7	1.31E-6	3.74E-6
Breast Cancer															
MCF7	0.335	1.832	1.701	.	1.485	0.171	0.170	91	.	77	-49	-49	1.63E-6	4.08E-6	> 1.00E-4
MDA-MB-231/ATCC	0.577	1.363	1.344	.	1.362	0.085	0.072	98	.	100	-85	-88	1.86E-6	3.46E-6	6.44E-6
HS 578T	0.733	1.350	1.345	.	1.297	0.570	0.636	99	.	91	-22	-13	2.31E-6	6.37E-6	> 1.00E-4
BT-549	0.750	1.510	1.452	.	1.523	0.038	0.036	92	.	102	-95	-95	1.83E-6	3.29E-6	5.91E-6
T-47D	0.672	1.502	1.479	.	1.267	0.417	0.541	97	.	72	-38	-19	1.58E-6	4.50E-6	> 1.00E-4
MDA-MB-468	0.587	1.366	1.314	.	0.726	0.058	0.021	93	.	18	-90	-97	1.40E-7	1.46E-6	4.25E-6

(B) Complex **8a.**

National Cancer Institute Developmental Therapeutics Program
In-Vitro Testing Results

NSC : D - 756777 / 1	Experiment ID : 1105NS53	Test Type : 08	Units : Molar
Report Date : July 15, 2011	Test Date : May 23, 2011	QNS :	MC :
COMI : MW03 (103478)	Stain Reagent : SRB Dual-Pass Related	SSPL : 0Y4T	

			Log10 Concentration												
	Time		Mean Optical Densities					Percent Growth							
Panel/Cell Line	Zero	Ctrl	-8.0	-7.0	-6.0	-5.0	-4.0	-8.0	-7.0	-6.0	-5.0	-4.0	GI50	TGI	LC50
Leukemia															
CCRF-CEM	0.527	1.797	1.814	1.758	1.172	0.337	0.306	101	97	51	-36	-42	1.02E-6	3.84E-6	> 1.00E-4
HL-60(TB)	0.594	2.542	2.318	2.493	1.692	0.390	0.352	88	97	56	-34	-41	1.18E-6	4.18E-6	> 1.00E-4
K-562	0.249	1.905	1.843	1.769	0.621	0.176	0.205	96	92	22	-30	-18	4.00E-7	2.70E-6	> 1.00E-4
MOLT-4	0.587	2.171	2.202	2.112	1.921	0.512	0.557	102	96	84	-13	-5	2.25E-6	7.38E-6	> 1.00E-4
RPMI-8226	0.789	2.492	2.520	2.454	2.144	0.435	0.582	102	98	80	-45	-26	1.73E-6	4.36E-6	> 1.00E-4
SR	0.346	1.612	1.626	1.612	1.090	0.310	0.308	101	100	59	-10	-11	1.34E-6	7.07E-6	> 1.00E-4
Non-Small Cell Lung Cancer															
A549/ATCC	0.315	1.519	1.456	1.427	1.398	0.289	0.169	95	92	90	-8	-47	2.55E-6	8.24E-6	> 1.00E-4
EKVX	0.746	1.651	1.615	1.594	1.576	0.048	0.060	96	94	92	-94	-92	1.68E-6	3.12E-6	5.81E-6
HOP-62	0.348	1.153	1.119	1.119	1.125	0.217	0.217	96	96	97	-38	-38	2.22E-6	5.24E-6	> 1.00E-4
NCI-H226	0.605	1.769	1.626	1.513	1.491	0.115	0.301	88	78	76	-81	-50	1.47E-6	3.05E-6	6.35E-6
NCI-H23	0.538	1.497	1.441	1.447	1.352	0.112	0.306	94	95	85	-79	-43	1.63E-6	3.29E-6	.
NCI-H322M	0.821	1.553	1.554	1.506	1.615	1.053	0.023	100	93	108	32	-97	5.76E-6	1.76E-5	4.30E-5
NCI-H460	0.226	1.940	1.947	1.874	1.811	0.146	0.132	100	96	92	-35	-42	2.15E-6	5.29E-6	> 1.00E-4
NCI-H522	0.593	1.555	1.481	1.427	0.781	0.103	0.244	92	87	20	-83	-59	3.52E-7	1.55E-6	4.79E-6
Colon Cancer															
COLO 205	0.270	1.389	1.460	1.505	0.888	0.147	0.200	106	110	55	-46	-26	1.13E-6	3.53E-6	> 1.00E-4
HCC-2998	0.685	2.505	2.453	2.422	2.452	0.255	0.092	97	95	97	-63	-87	1.97E-6	4.05E-6	8.31E-6
HCT-116	0.186	1.172	1.144	1.153	0.572	0.027	0.036	97	98	39	-85	-81	6.53E-7	2.06E-6	5.19E-6
HCT-15	0.472	2.207	2.056	2.090	2.022	0.091	0.143	91	93	89	-81	-70	1.70E-6	3.35E-6	6.60E-6
HT29	0.217	1.162	1.177	1.151	1.003	0.088	0.157	102	99	83	-60	-28	1.71E-6	3.82E-6	.
KM12	0.439	1.960	1.945	1.883	1.973	0.538	0.048	99	95	101	7	-89	3.46E-6	1.17E-5	3.90E-5
SW-620	0.228	1.430	1.396	1.433	0.660	0.066	0.118	97	100	36	-71	-48	6.04E-7	2.17E-6	.
CNS Cancer															
SF-268	0.469	1.576	1.507	1.492	1.530	0.061	0.107	94	92	96	-87	-77	1.78E-6	3.34E-6	6.28E-6
SF-295	0.640	2.022	1.971	1.964	1.812	0.906	0.048	96	96	85	19	-93	3.40E-6	1.49E-5	4.17E-5
SF-539	0.834	2.023	2.049	2.065	2.153	0.091	0.528	102	104	111	-89	-37	2.02E-6	3.58E-6	.
SNB-19	0.448	1.322	1.239	1.242	1.282	0.162	0.036	91	91	95	-64	-92	1.93E-6	3.97E-6	8.18E-6
SNB-75	0.603	1.258	1.201	1.169	1.235	0.041	0.422	91	86	96	-93	-30	1.76E-6	3.22E-6	.
U251	0.254	1.219	1.225	1.172	0.692	0.015	0.094	101	95	45	-94	-63	8.07E-7	2.11E-6	4.82E-6
Melanoma															
LOX IMVI	0.221	1.540	1.528	1.502	1.018	0.015	0.087	99	97	60	-93	-61	1.17E-6	2.47E-6	5.22E-6
MALME-3M	0.694	1.455	1.419	1.449	1.177	0.133	0.444	95	99	63	-81	-36	1.24E-6	2.75E-6	.
M14	0.393	1.250	1.248	1.264	1.225	0.046	0.111	100	102	97	-88	-72	1.79E-6	3.34E-6	6.21E-6
MDA-MB-435	0.445	2.002	1.980	1.909	1.853	0.052	0.257	99	94	90	-88	-42	1.68E-6	3.21E-6	.
SK-MEL-2	0.990	1.623	1.605	1.601	1.648	0.262	0.666	97	97	104	-74	-33	2.01E-6	3.85E-6	.
SK-MEL-28	0.516	1.438	1.424	1.437	1.263	0.089	0.339	99	100	81	-83	-34	1.55E-6	3.12E-6	.
SK-MEL-5	0.442	2.944	2.902	2.725	2.792	0.457	0.018	98	91	94	1	-96	2.95E-6	1.01E-5	3.34E-5
UACC-257	0.776	1.468	1.477	1.425	1.347	0.097	0.235	101	94	83	-88	-70	1.55E-6	3.06E-6	6.01E-6
UACC-62	0.834	2.267	2.240	2.177	2.080	0.085	0.071	98	94	87	-90	-91	1.62E-6	3.10E-6	5.95E-6
Ovarian Cancer															
IGROV1	0.523	1.703	1.716	1.672	1.735	0.130	0.417	101	97	103	-75	-20	1.98E-6	3.78E-6	.
OVCAR-3	0.499	1.309	1.353	1.319	1.112	0.010	0.012	105	101	76	-98	-98	1.40E-6	2.73E-6	5.29E-6
OVCAR-4	0.488	1.486	1.454	1.506	1.279	0.036	0.306	97	102	79	-93	-37	1.48E-6	2.89E-6	.
OVCAR-5	0.573	1.500	1.487	1.444	1.453	0.097	0.129	99	94	95	-83	-78	1.79E-6	3.41E-6	6.51E-6
OVCAR-8	0.386	1.457	1.479	1.450	1.211	0.103	0.391	102	99	77	-73	.	1.51E-6	.	.
NCI/ADR-RES	0.452	1.286	1.301	1.263	1.286	0.529	0.355	102	97	100	9	-22	3.55E-6	1.99E-5	> 1.00E-4
SK-OV-3	0.503	1.485	1.489	1.474	1.506	0.950	0.048	100	99	102	45	-91	8.32E-6	2.16E-5	5.03E-5
Renal Cancer															
786-0	0.533	1.930	1.841	1.815	1.866	0.014	0.046	94	92	95	-97	-91	1.72E-6	3.13E-6	5.68E-6
A498	1.239	2.101	2.005	2.013	1.986	1.528	0.003	89	90	87	33	-100	4.89E-6	1.78E-5	4.23E-5
ACHN	0.418	1.393	1.394	1.400	1.118	0.015	0.025	100	101	72	-97	-94	1.35E-6	2.67E-6	5.29E-6
CAKI-1	0.688	2.077	2.044	2.041	1.874	0.153	0.323	98	97	85	-78	-53	1.65E-6	3.34E-6	6.75E-6
RXF 393	0.541	1.188	1.188	1.085	1.043	-0.005	-0.011	100	84	77	-100	-100	1.43E-6	2.73E-6	5.23E-6
SN12C	0.583	1.829	1.819	1.764	1.653	0.339	0.510	99	95	86	-42	-13	1.91E-6	4.70E-6	> 1.00E-4
TK-10	0.657	1.150	1.103	1.076	1.039	0.015	0.019	90	85	77	-98	-97	1.43E-6	2.77E-6	5.34E-6
UO-31	0.566	1.611	1.544	1.543	1.504	0.018	0.014	94	93	90	-97	-98	1.63E-6	3.02E-6	5.61E-6
Prostate Cancer															
PC-3	0.488	1.158	1.134	1.108	1.006	0.059	0.159	96	93	77	-88	-67	1.46E-6	2.93E-6	5.89E-6
DU-145	0.300	1.186	1.174	1.187	1.165	0.007	.	99	100	98	-98	-100	1.75E-6	3.16E-6	5.69E-6
Breast Cancer															
MCF7	0.335	1.807	1.738	1.711	1.432	0.220	0.160	95	93	75	-34	-52	1.68E-6	4.84E-6	7.38E-5
MDA-MB-231/ATCC	0.577	1.406	1.420	1.345	1.401	0.074	0.160	102	93	99	-87	-72	1.84E-6	3.41E-6	6.32E-6
HS 578T	0.733	1.451	1.427	1.466	1.397	0.634	0.687	97	102	92	-14	-6	2.51E-6	7.46E-6	> 1.00E-4
BT-549	0.750	1.548	1.509	1.471	1.591	0.017	0.060	95	90	105	-98	-92	1.87E-6	3.30E-6	5.82E-6
T-47D	0.672	1.648	1.543	1.633	1.199	0.561	0.696	89	98	54	-17	2	1.14E-6	.	> 1.00E-4
MDA-MB-468	0.587	1.410	1.338	1.164	0.761	0.111	0.090	91	70	21	-81	-85	2.57E-7	1.61E-6	4.97E-6

Table S2

COMPARE results using NCI/DTP synthetic agents database for the GI_{50} endpoint

8			8a		
Correlated agent	**PCC**	**Mechanism**	**Correlated agent**	**PCC**	**Mechanism**
MW03	0.868	-	MW02	0.868	-
Pleurotin	0.661	Inhibit flavoproteinthioredoxin reductase Inhibits hypoxia induced increase of HIF-1a	Eupacunoxin	0.673	
Mercaptoacetate	0.654	Potential DNA cleavage	Bipinnatin H	0.664	
Zinolide	0.652	No data on MoA	Mercaptoacetate	0.664	Potential DNA cleavage
Xestoquinone	0.649	Topo II mediated DNA cleavage	Urdamycin A, pentaacetate	0.659	
Cryptosporiopsin	0.649	Inhibit RNA synthesis by altering nucleotides. Also disrupts production of ATP.	Arnebin 1	0.658	
Methyl-CCNU	0.642	Alkylating agent	Mikanolide	0.656	
Eupacurvin	0.636	No data on MoA	Multistatin	0.652	
Urdamycin A, pentaacetate	0.614		Gold, chloro(triethyl phosphine)	0.65	
Homopterocarpin	0.605		Straital B	0.65	
			Acnistin F	0.648	
			Cryptosporiosin	0.647	Inhibit RNA synthesis by altering nucleotides. Also disrupts production of ATP.
			Heliangolide	0.645	
			Eupacurvin	0.645	
			Withaferin A	0.643	

NCI/DTP database. Only those agents returned within the first 100 correlations, with (PCC) > 0.6 are shown. Agents with compound names, and not registered names, are omitted.

Table S3

COMPARE results using NCI/DTP synthetic agents database for the TGI endpoint

8			**8a**		
Correlated agent	**PCC**	**Mechanism**	**Correlated agent**	**PCC**	**Mechanism**
MW03	0.945	-	MW02	0.874	-
Mercaptoacetate	0.656	Potential DNA cleavage	Mercaptoacetate	0.695	Potential DNA cleavage
			Gold, chloro(triethyl phosphine)	0.638	
			Arnebin 1	0.614	
			Straital B	0.610	
			Santolinapolyacetaylene 18	0.602	

NCI/DTP database. Only those agents returned within the first 100 correlations, with PCC > 0.6 are shown. Agents with only their compound structure name, and not registered names, are omitted.

Table S4

COMPARE results using the NCI/DTP synthetic agents database for the LC_{50} endpoint

8			8a		
Correlated agent	**PCC**	**Mechanism**	**Correlated agent**	**PCC**	**Mechanism**
MW03	0.942	-	MW02	0.942	-
Withaferin A	0.847				
Mercaptoacetate	0.809	Potential DNA cleavage	Withaferin A	0.73	
Urdamycin A, pentacetate	0.793		Longikaurin B	0.727	
Kalafungin(USAN)	0.785		Eupachlorin acetate	0.727	
T 1(VAN)	0.773		Cumertilin	0.723	
Longikaurin B	0.765		Celastrol	0.684	
Stannane, dibutyldithiocyanato	0.761		Acetyl rolandrolide	0.682	
Cumertilin	0.739		Iso-withanolide E 14,15-epoxy-6 alpha	0.662	
Helenine	0.736		Alpha-bromochalcone	0.653	
ChelerythrineHCl	0.73		Cleandrin	0.653	
Secalone B	0.726		Arylpurine derivatives	0.65	
Farinosin, dehydro	0.72				
Plumbaein	0.715				
Celastrol	0.712				
Sanguinarine Nitrate	0.71				

NCI/DTP database. Only those agents returned within the first 100 correlations, with PCC > 0.6 are shown. Agents with compound names, and not registered names, are omitted.

Table S5

Values for the cell cycle analysis using flow cytometry experiments in A2780 ovarian cancer cells. All values are compared to the untreated controls for statistical significance calculations.

Sample	Cell cycle	Averages	Stdev	P-value against -ve
Controls	Sub-G1	0.000	0.000	
	G1	62.700	0.854	
	S	23.167	0.751	
	G2/M	10.703	0.362	
Colchicine (100 nM)	Sub-G1	12.400	0.436	0.000411643
	G1	7.553	0.832	1.46989E-07
	S	13.433	0.551	0.000100684
	G2/M	55.933	2.325	0.000683922
Taxol (100 nM)	Sub-G1	22.933	1.701	0.001828733
	G1	17.300	1.153	1.66939E-06
	S	11.433	0.907	8.43193E-05
	G2/M	45.600	1.473	0.000306016
7 (2 µM)	Sub-G1	3.305	0.601	0.081418053
	G1	57.950	0.636	0.007032042
	S	29.000	0.849	0.014886727
	G2/M	15.050	0.778	0.051306728
7a (2 µM)	Sub-G1	4.360	0.740	0.00946604
	G1	46.533	3.647	0.012960242
	S	30.300	1.114	0.001410555
	G2/M	20.033	2.470	0.020725302
8 (2 µM)	Sub-G1	13.750	0.354	0.01157363
	G1	54.500	0.283	0.001328262
	S	17.950	0.778	0.013337581
	G2/M	17.300	0.566	0.011716941
8a (2 µM)	Sub-G1	2.683	0.163	0.001221477
	G1	56.600	0.624	0.000870273
	S	22.667	1.026	0.536401588
	G2/M	16.700	1.253	0.009689256

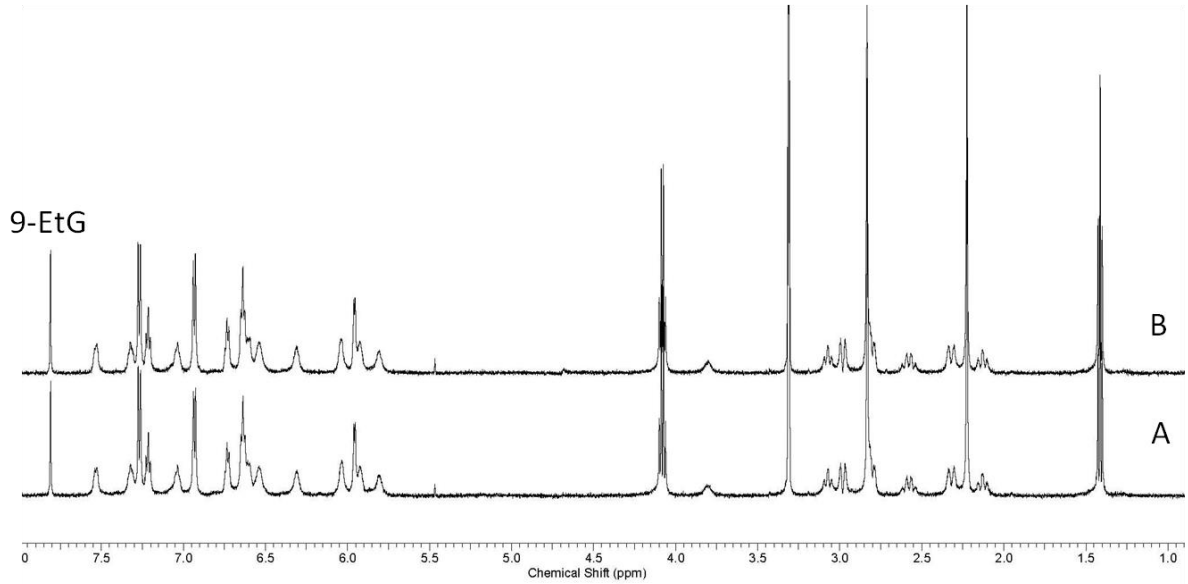

Figure S1. ^{1}H NMR spectra of **8a** (1.5 mM) and 9-EtG (1.5 mM) in 25% MeOD-d_4/75% D_2O (v/v) at 310 K after (A) 10 min and (B) 24 h.

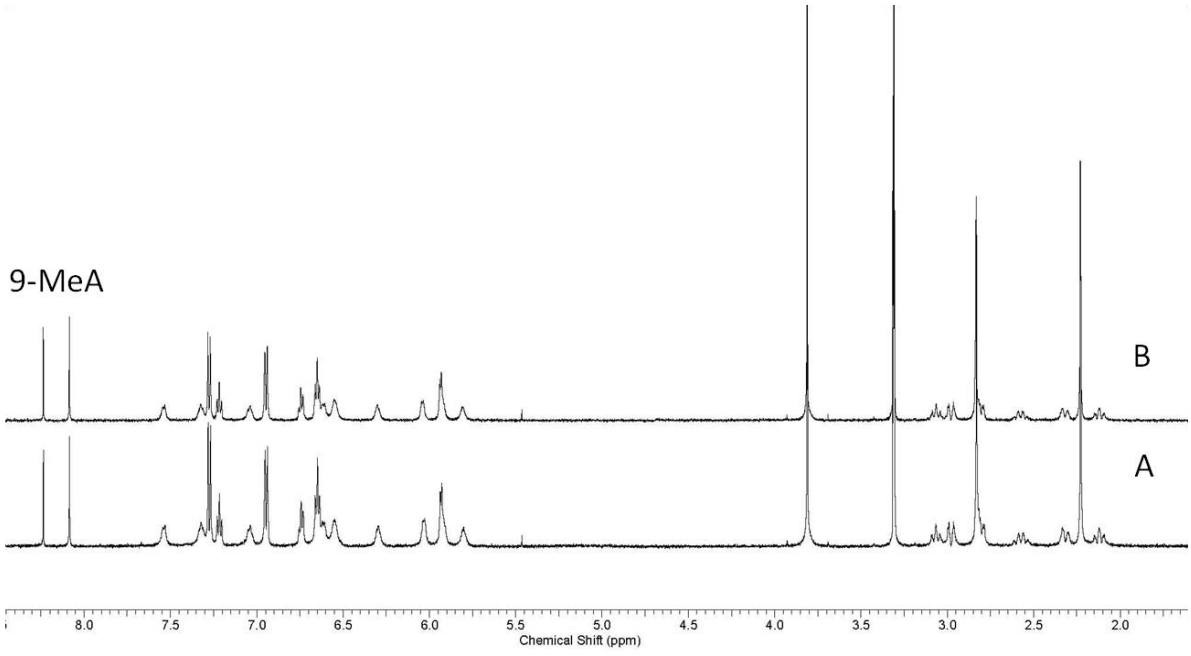

Figure S2. ^{1}H NMR spectra of **8a** (1.5 mM) and 9-MeA (1.5 mM) in 25% MeOD-d_4/75% D_2O (v/v) at 310 K after (A) 10 min and (B) 24 h.

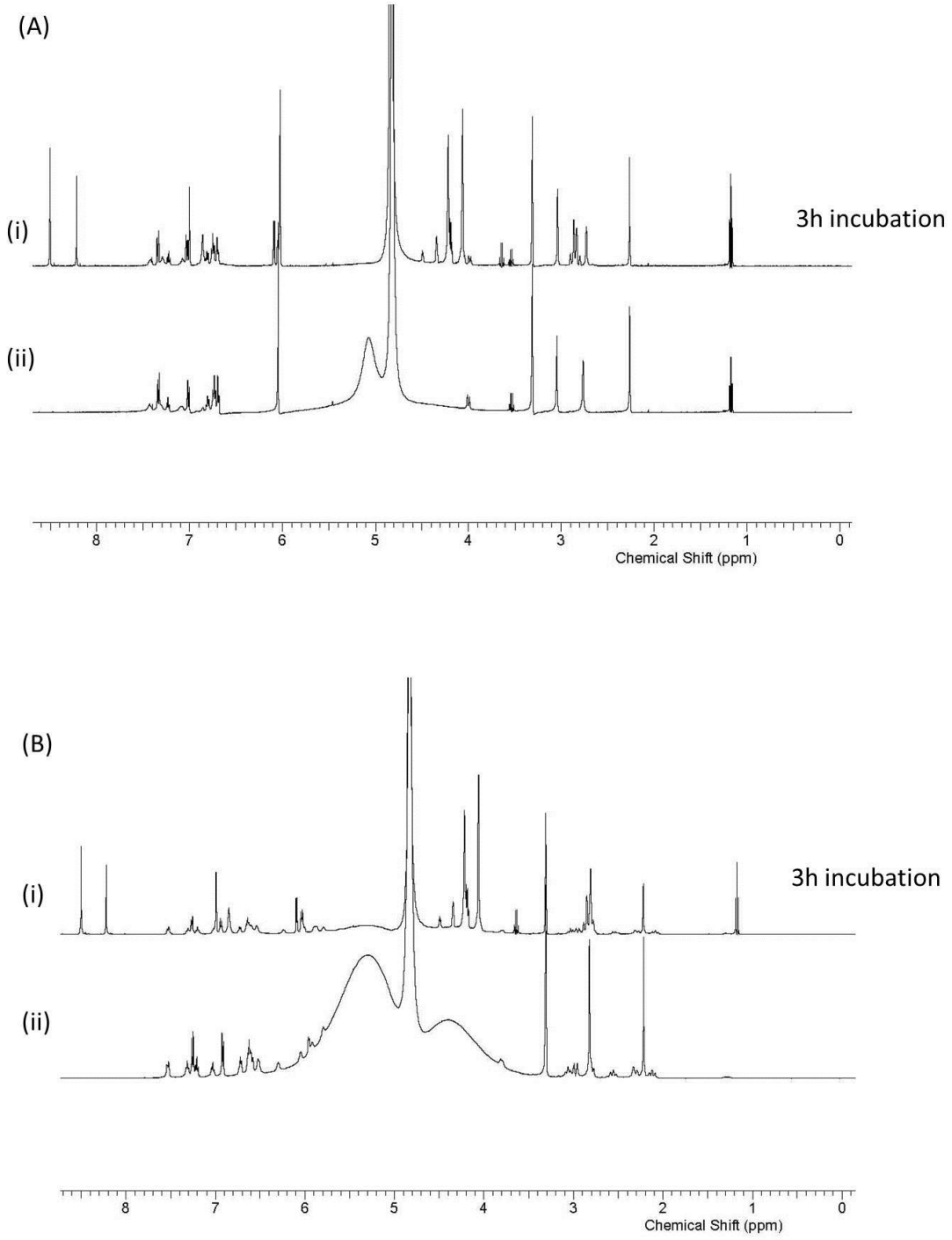

Figure S3. ^{1}H NMR spectra of **7** (A) and **8a** (B) with NADH in 25% MeOD-d_4/75% D_2O (v/v) at 298 K: (i) equilibrium solution of the complexes (1.5 mM); (ii) 3 h after addition of 3 mol equiv of NADH to the above solution. No reaction between the complexes and NADH was observed after 3 h incubation. The broad humps in (ii) arise from incomplete H_2O peak suppression.

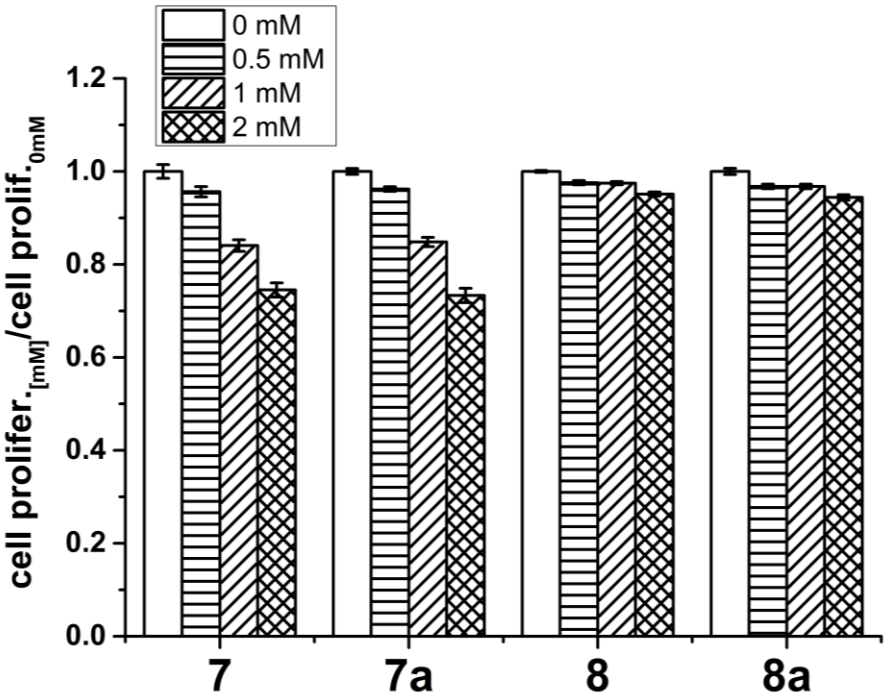

Figure S4. Effect of co-administration of sodium formate (0, 0.5, 1 or 2 mM) and complexes **7/8** (1/5 IC_{50}) on cell survival.

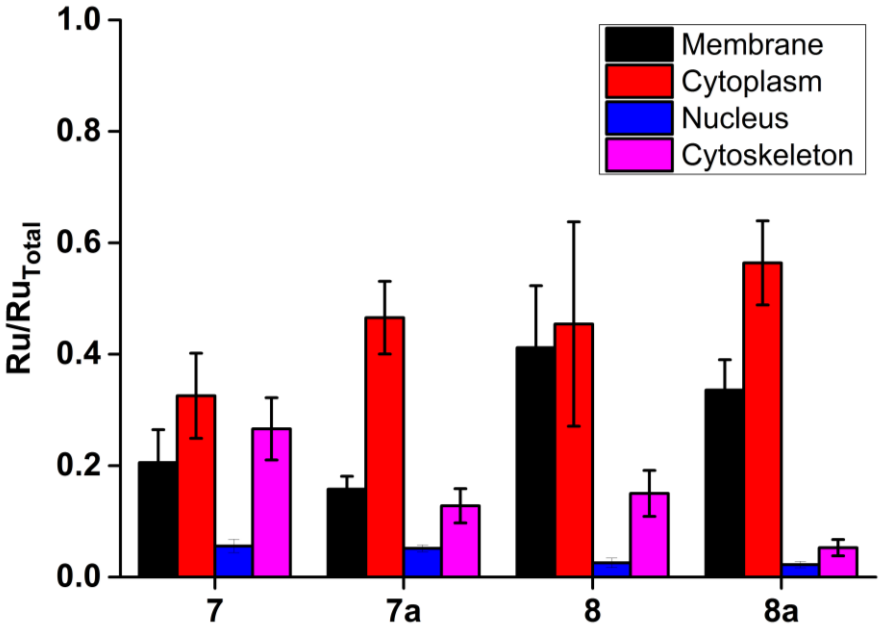

Figure S5. Relative distribution of ruthenium in the different cellular fractions of A2780 ovarian carcinoma cells (expressed in ng Ru/million cells) after 24 h treatment with 2 µM of **7/8**.

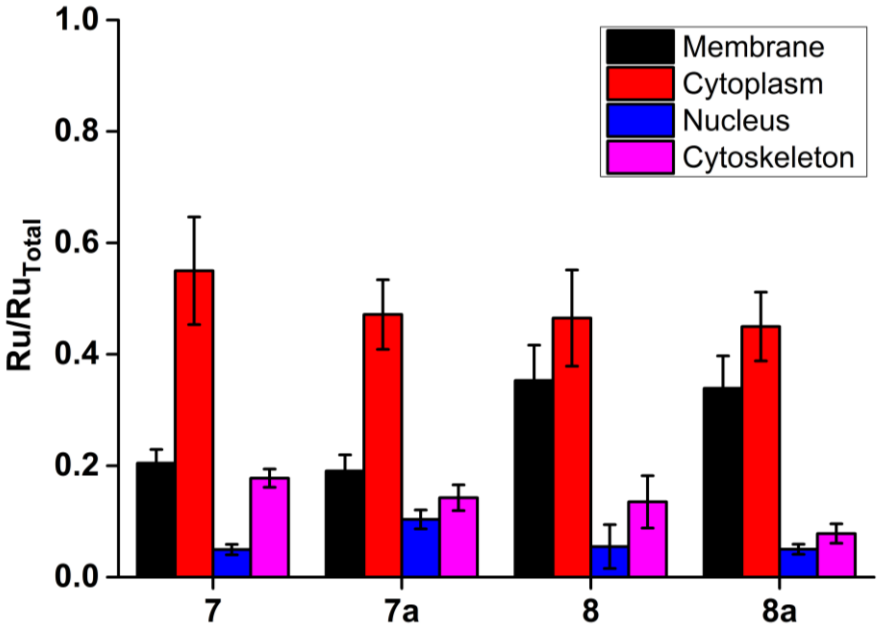

Figure S6. Relative distribution of ruthenium in the different cellular fractions of A2780 ovarian carcinoma cells (expressed in ng Ru/million cells) after 24 h treatment with IC_{50} concentration of **7/8**.

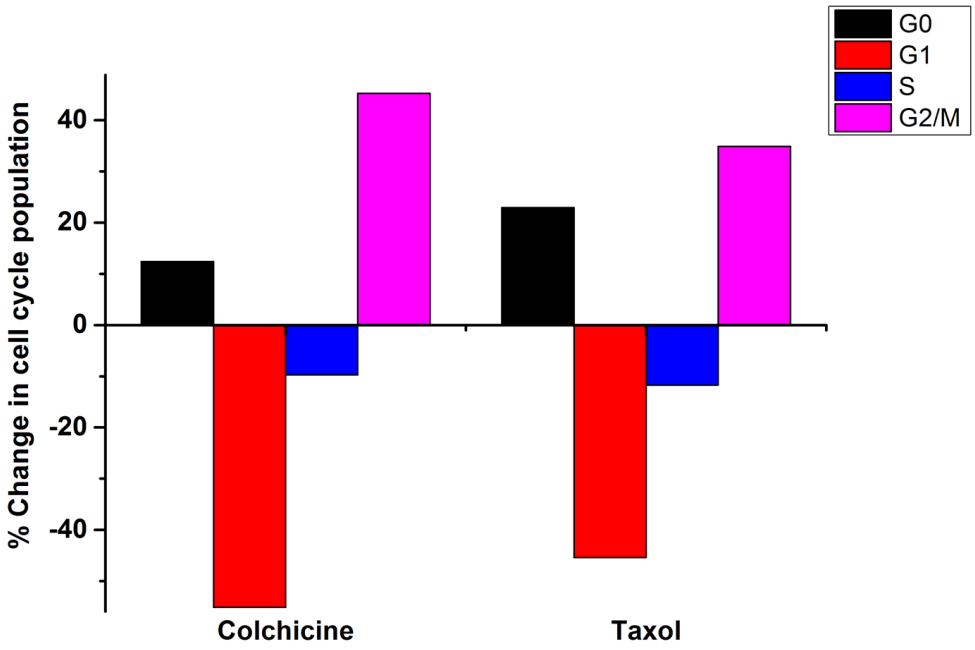

Figure S7. Changes in the cell cycle of A2780 ovarian carcinoma cells after 24 h treatment with 100 nM of Colchicine or Taxol.

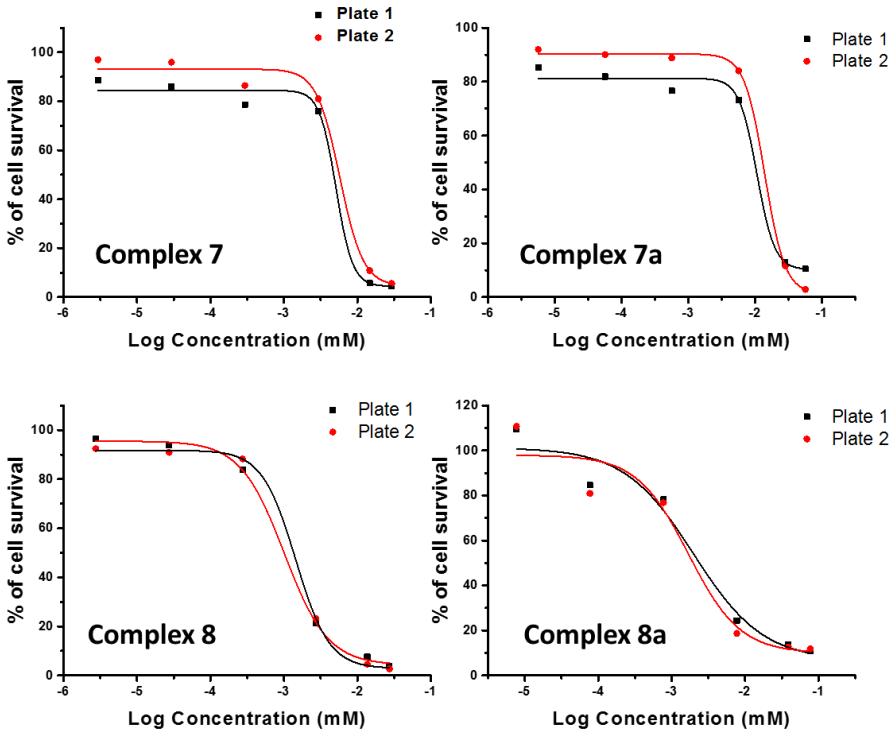

Figure S8. Cell viability test of A2780 ovarian carcinoma cells treated with ruthenium complexes (7, 7a, 8, 8a).

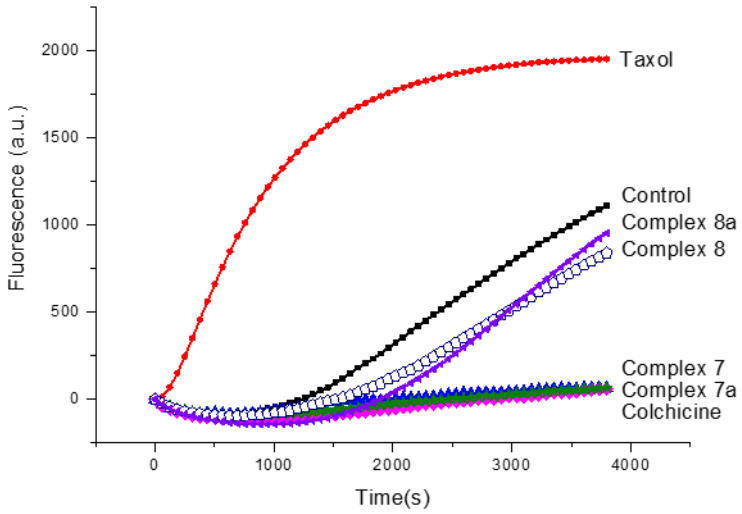

Figure S9. Kinetics of tubulin polymerisation at 310 K : untreated (▬■▬), complex **7** (▬◆▬, 10 µM), complex **7a** (▬★▬, 10 µM), complex **8** (▬⬠▬, 10 µM), complex **8a** (▬◀▬, 10 µM), Taxol (▬●▬, 3 µM, stabilises microtubules) and Colchicine (▬▲▬, 3 µM, inhibits microtubule formation). Microtubule formation was monitored by the increase in fluorescence (arbitrary units) of a reporter incorporated into microtubules as polymerisation proceeds.