Supplementary materials

The influence of stereochemistry on the biological activity of metal complexes with terpene ligands. I. Antitumor activity of unichiral palladium complexes based on *L*- and *D*-camphor benzyl imines

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Table S1. *In silico* prediction of cytotoxicity of **HL1**, **HL2** and palladium complexes **1-3**

(+)-**HL1** / (–)-**HL1**			
Pa[a]	**Pi**[b]	**Description**	
0.605	0.109	A2780cisR	Cisplatin-resistant ovarian carcinoma
0.370	0.153	DU-4475	Breast Carcinoma
0.330	0.026	H9c2	Rat DB1X heart myoblast cell line
0.329	0.042	HepG2-CD81	Hepatoblastoma (HepG2) cells expressing CD81
0.317	0.059	MKN-74	Gastric tubular adenocarcinoma
0.309	0.082	8505C	Thyroid gland undifferentiated (anaplastic) carcinoma
(+)-**HL2** / (–)-**HL2**			
Pa	**Pi**	**Description**	
0.726	0.058	A2780cisR	Cisplatin-resistant ovarian carcinoma
0.393	0.121	DU-4475	Breast Carcinoma
0.355	0.018	H9c2	Rat DB1X heart myoblast cell line
0.350	0.087	MDA-MB-231	Breast adenocarcinoma
0.343	0.038	HepG2-CD81	Hepatoblastoma (HepG2) cells expressing CD81
0.343	0.043	U-266	Plasma cell myeloma
0.338	0.041	MKN-74	Gastric tubular adenocarcinoma
0.321	0.068	8505C	Thyroid gland undifferentiated (anaplastic) carcinoma
0.314	0.046	HOP-18	Non-small cell lung carcinoma
(+)-**1** / (–)-**1**			
Pa	**Pi**	**Description**	
0.772	0.042	A2780cisR	Cisplatin-resistant ovarian carcinoma
0.634	0.005	M19-MEL	Melanoma

0.473	0.048	DU-4475	Breast Carcinoma
0.467	0.011	HOP-18	Non-small cell lung carcinoma
0.462	0.049	GIST430	Gastrointestinal stromal tumor
0.456	0.045	OPM-2	Plasma cell myeloma
0.413	0.041	EKVX	Non-small cell lung carcinoma
0.402	0.013	MKN-74	Gastric tubular adenocarcinoma
0.364	0.037	HCC1806	Acantholytic Squamous Cell Carcinoma
0.336	0.051	8505C	Thyroid gland undifferentiated (anaplastic) carcinoma
0.315	0.033	H9c2	Rat DB1X heart myoblast cell line
0.313	0.051	RCC4	Clear cell renal cell carcinoma
0.311	0.073	OVCAR-5	Ovarian adenocarcinoma
0.302	0.015	NCI/ADR-RES	High grade ovarian serous adenocarcinoma
0.302	0.082	SK-MEL-2	Melanoma
(+)-**2** / (–)-**2**			
Pa	**Pi**	**Description**	
0.714	0.063	A2780cisR	Cisplatin-resistant ovarian carcinoma
0.425	0.086	DU-4475	Breast Carcinoma
0.374	0.021	MKN-74	Gastric tubular adenocarcinoma
0.371	0.108	SK-MEL-1	Metastatic melanoma
0.361	0.016	H9c2	Rat DB1X heart myoblast cell line
0.354	0.065	M19-MEL	Melanoma
0.343	0.038	HepG2-CD81	Hepatoblastoma (HepG2) cells expressing CD81
0.333	0.039	HOP-18	Non-small cell lung carcinoma
0.332	0.057	8505C	Thyroid gland undifferentiated (anaplastic) carcinoma
0.326	0.087	HCC1806	Acantholytic Squamous Cell Carcinoma
(+)-**3** / (–)-**3**			
Pa	**Pi**	**Description**	
0.844	0.017	A2780cisR	Cisplatin-resistant ovarian carcinoma
0.632	0.005	M19-MEL	Melanoma
0.49	0.008	HOP-18	Non-small cell lung carcinoma

0.482	0.027	EKVX	Non-small cell lung carcinoma
0.478	0.02	RXF393	Renal cell carcinoma
0.459	0.029	HCC2998	Colon adenocarcinoma
0.456	0.109	MCF7	Breast carcinoma
0.453	0.062	DU-4475	Breast Carcinoma
0.448	0.031	SF-295	Glioblastoma
0.446	0.032	SK-MEL-2	Melanoma
0.442	0.027	NCI-H522	Non-small cell lung carcinoma
0.439	0.031	KM12	Colon adenocarcinoma
0.433	0.023	SK-MEL-5	Melanoma
0.433	0.024	Hs-578T	Invasive ductal breast carcinoma
0.411	0.008	H9c2	Rat DB1X heart myoblast cell line
0.407	0.035	SF-268	Glioblastoma
0.404	0.036	UO-31	Renal carcinoma
0.39	0.015	MKN-74	Gastric tubular adenocarcinoma
0.385	0.034	OVCAR-8	Ovarian adenocarcinoma
0.375	0.046	786-0	Renal carcinoma
0.372	0.038	OVCAR-3	Ovarian adenocarcinoma
0.363	0.039	SF-539	Glioblastoma
0.356	0.011	NCI/ADR-RES	High grade ovarian serous adenocarcinoma
0.344	0.007	SNB-19	Astrocytoma
0.344	0.06	OVCAR-5	Ovarian adenocarcinoma
0.341	0.046	8505C	Thyroid gland undifferentiated (anaplastic) carcinoma
0.34	0.01	MDA-MB-435	Amelanotic melanoma
0.334	0.053	NCI-H226	Non-small cell lung carcinoma
0.334	0.072	HCC1806	Acantholytic Squamous Cell Carcinoma
0.329	0.048	SR	Adult immunoblastic lymphoma
0.326	0.069	U-251	Astrocytoma

[a]Probability «be active».
[b]Probability «be inactive».