

### 3-Pyridinylidene derivatives of chemically modified lupane and ursane triterpenes as promising anticancer agents by targeting apoptosis

Oxana Kazakova<sup>1#\*</sup>, Codruța Șoica<sup>2,3#</sup>, Marat Babaev<sup>1</sup>, Anastasiya Petrova<sup>1</sup>, El'mira Khusnutdinova<sup>1</sup>, Alexander Poptsov<sup>1</sup>, Ioana Macașoi<sup>2,3</sup>, George Drăghici<sup>2,3</sup>, Ștefana Avram<sup>2,3</sup>, Lavinia Vlaia<sup>2,4</sup>, Alexandra Mioc<sup>2,3</sup>, Marius Mioc<sup>2,3\*</sup>, Cristina Dehelean<sup>2,3</sup>, Adrian Voicu<sup>5</sup>

<sup>1</sup>*Ufa Institute of Chemistry UFRS RAS, pr. Oktyabrya 71, 450054 Ufa, Russian Federation*

<sup>2</sup>*Faculty of Pharmacy, "Victor Babes" University of Medicine and Pharmacy, 2nd Eftimie Murgu Square, Timisoara, 300041, Romania*

<sup>3</sup>*Res. Ctr. Pharmacotoxicol Evaluat, Faculty of Pharmacy, "Victor Babes" University of Medicine and Pharmacy Timisoara, 2nd Eftimie Murgu Sq., Timisoara 300041, Romania;*

<sup>4</sup>*Res. Ctr. Drug Formulation and Technology, Faculty of Pharmacy, "Victor Babes" University of Medicine and Pharmacy Timisoara, 2nd Eftimie Murgu Sq., Timisoara 300041, Romania;*

<sup>5</sup>*Faculty of Medicine, "Victor Babes" University of Medicine and Pharmacy, 2nd Eftimie Murgu Sq., Timisoara 300041, Romania*

# Authors with equal contribution jointly sharing the position of first author

\* Corresponding authors: obf@anrb.ru, marius.mioc@umft.ro

#### Abstract

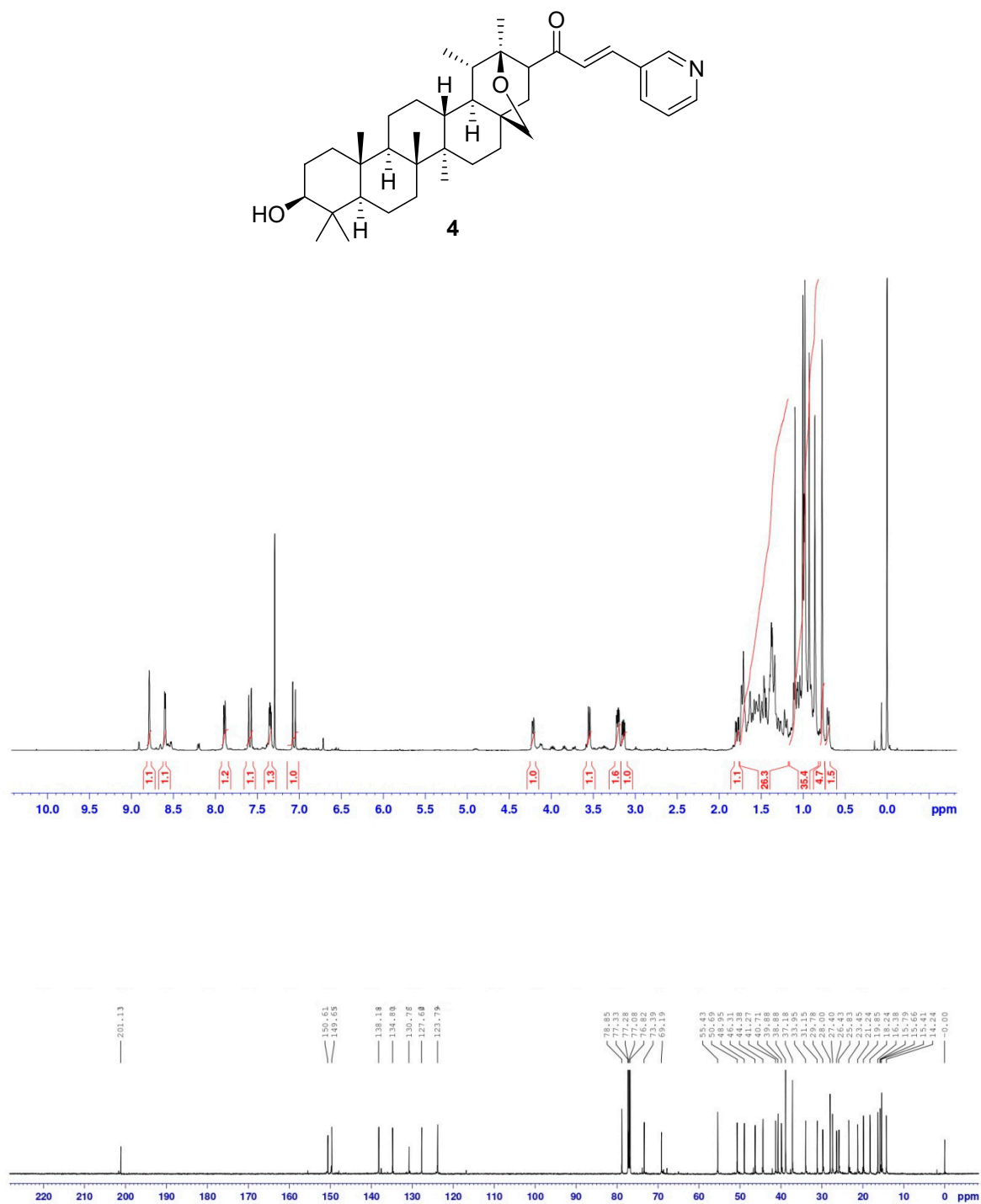
Cancer persists as a global challenge due to the extent to which conventional anticancer therapies pose high risks counterbalanced with their therapeutic benefit. Natural occurring substances stand as an important safer alternative source for anticancer drug development. In the current study a series of modified lupane and ursane derivatives was subjected to *in vitro* screening on the NCI-60 cancer cell line panel. Compounds **6** and **7** emerged as highly active with GI<sub>50</sub> values ranging from 0.03  $\mu$ M to 5.9  $\mu$ M for compound **6**, while compound **7** recorded GI<sub>50</sub> values between 0.18 – 1.53  $\mu$ M. Thus, these two compounds were further assessed in detail in order to identify a possible antiproliferative mechanism of action. DAPI staining revealed that both compounds induced nuclei condensation and overall cell morphological changes consistent with apoptotic cell death. rtPCR analysis showed that both compounds induced up-regulation of pro-apoptotic Bak and Bad genes while down-regulating Bcl-XL and Bcl-2 anti-apoptotic genes. Molecular docking analysis revealed that both compounds exhibited high scores for Bcl-XL inhibition, while compound **7** showed higher *in silico* Bcl-XL inhibition potential as compare to the native inhibitor ATB-737; suggesting that compounds may induce apoptotic cell death through targeted anti-apoptotic protein inhibition, as well.

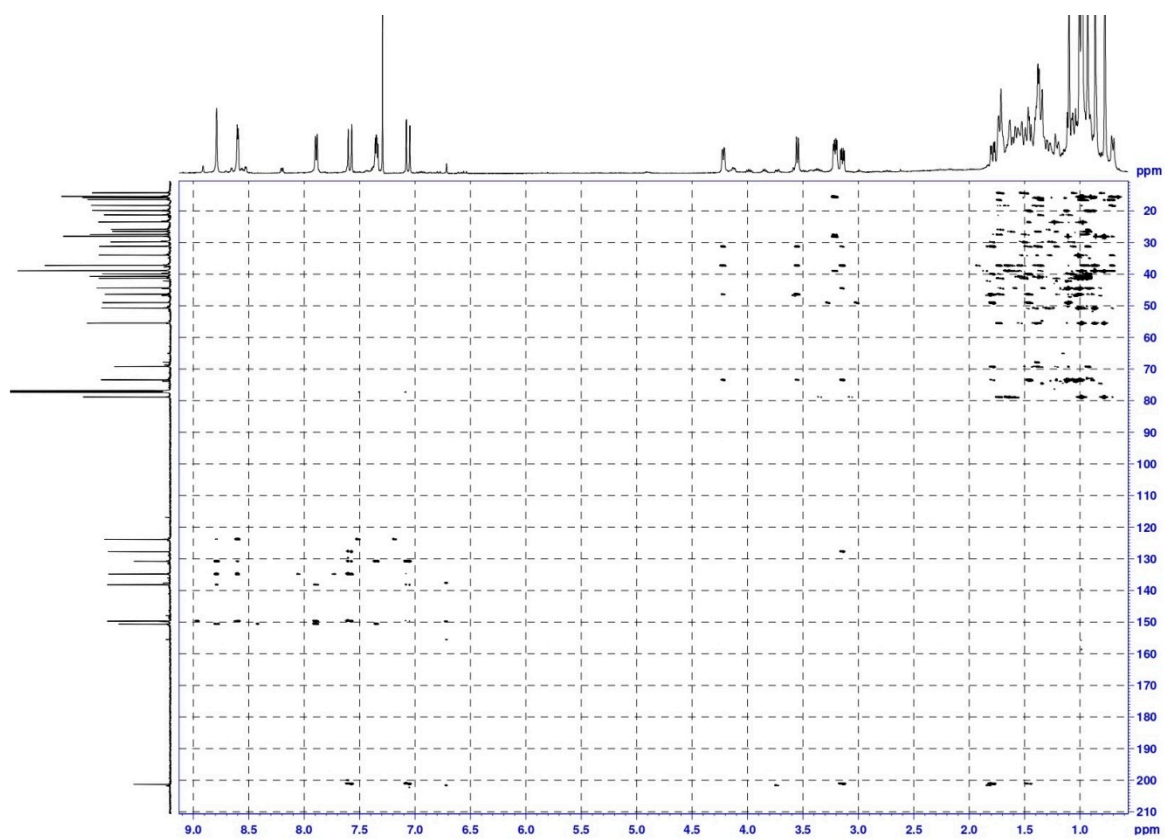
**Keywords:** pentacyclic triterpenes, platanoate, ursane, Claisen–Schmidt reaction, NCI-60, anticancer activity, apoptosis, antiangiogenic, molecular docking

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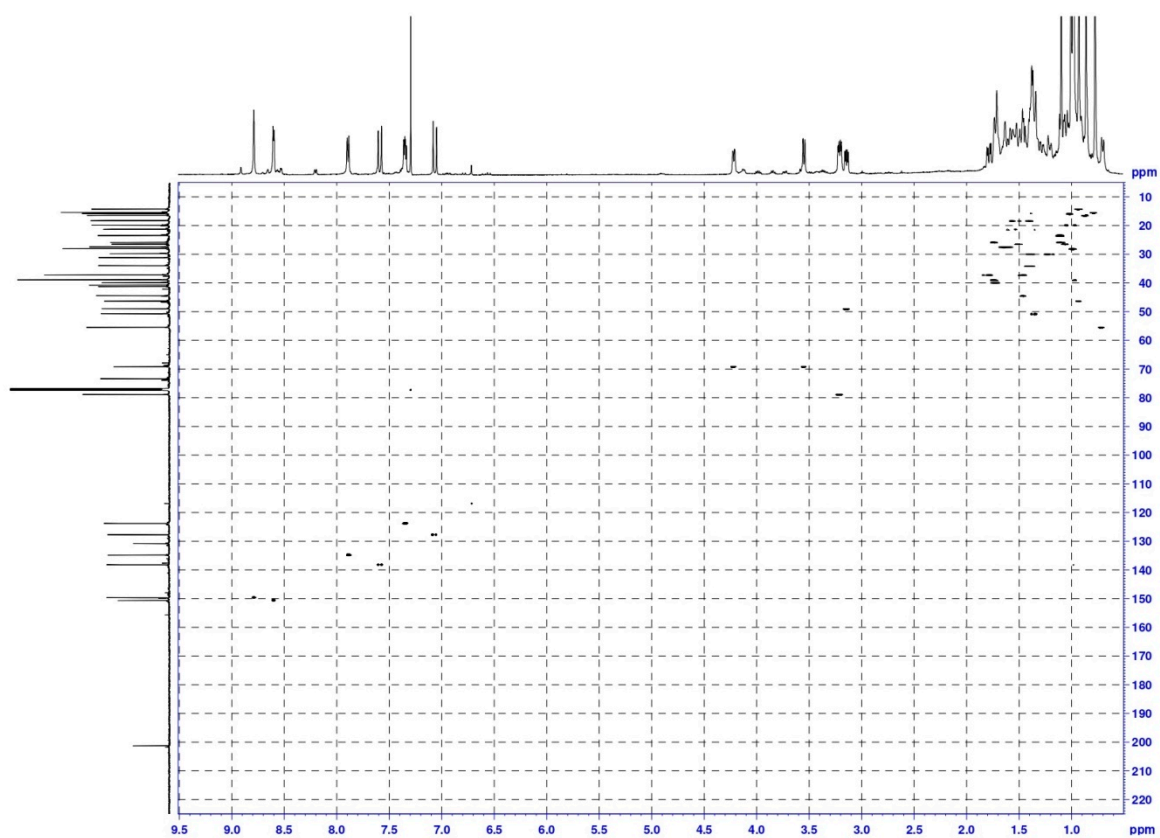
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**Figure S1.** NMR spectra of compound **4**



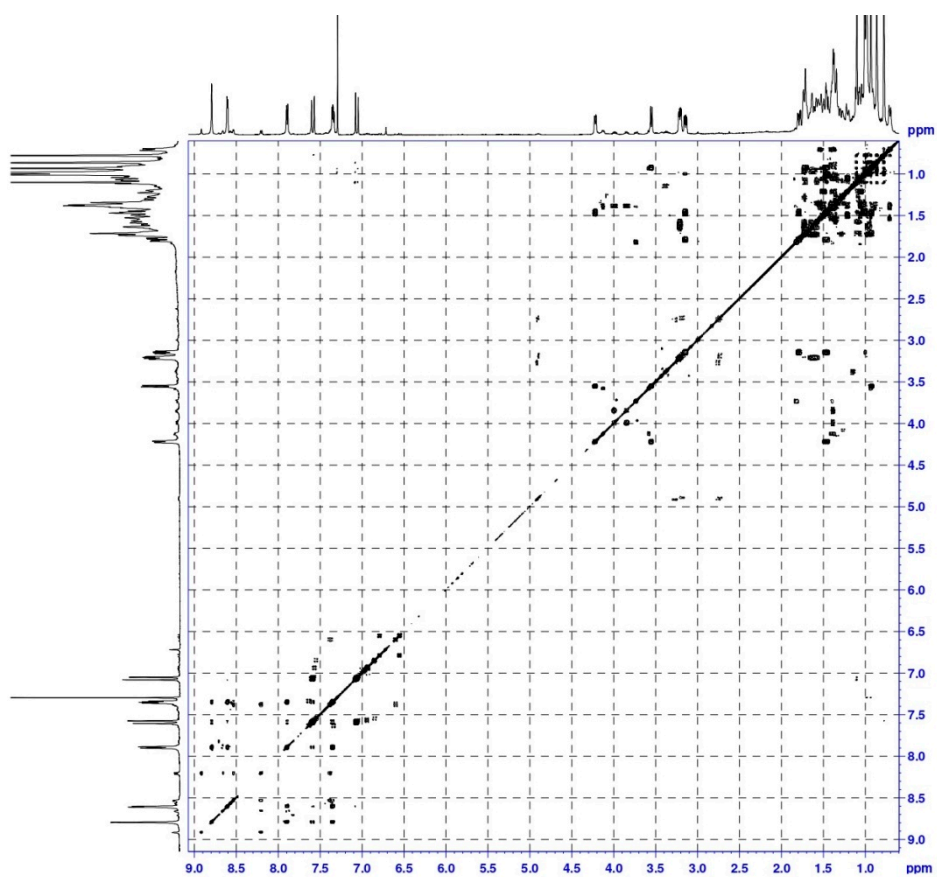


HMBC spectrum of compound 4

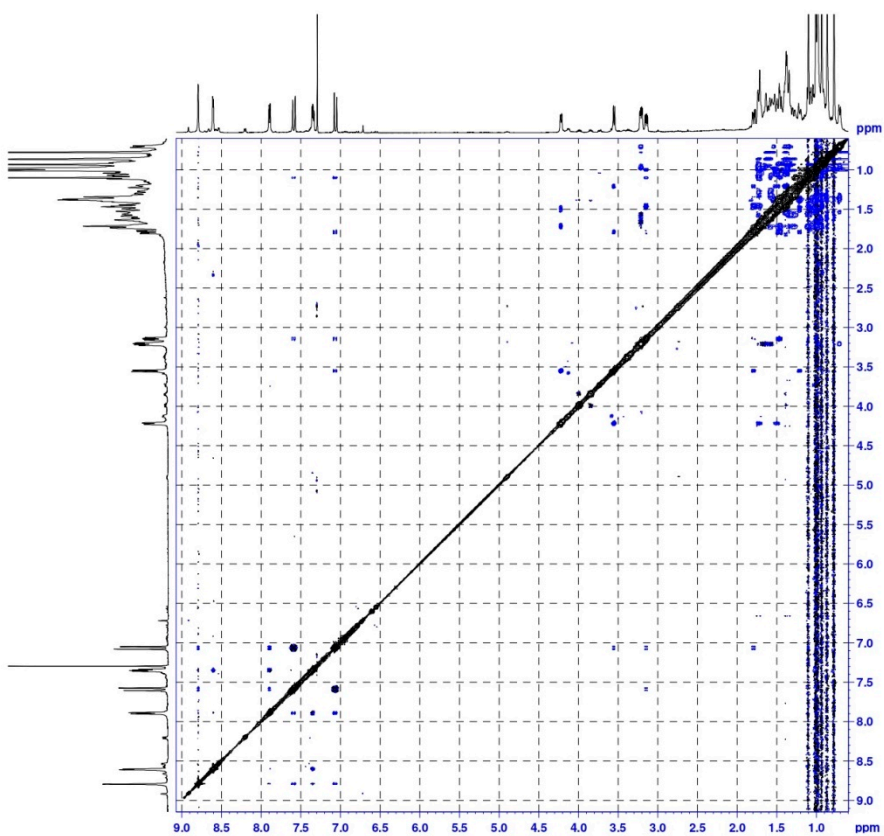


HSQC spectrum of compound 4



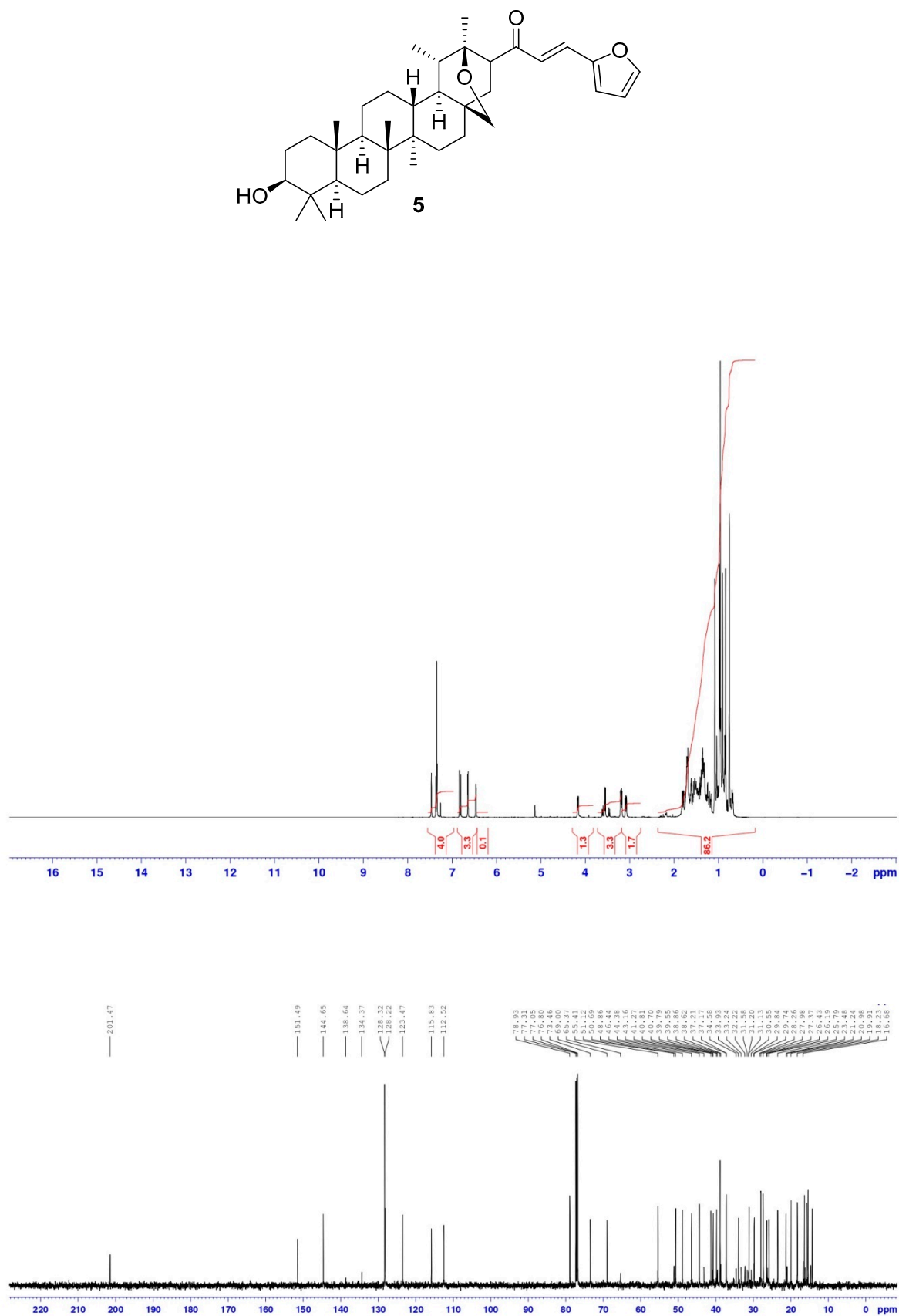


COSY spectrum of compound 4

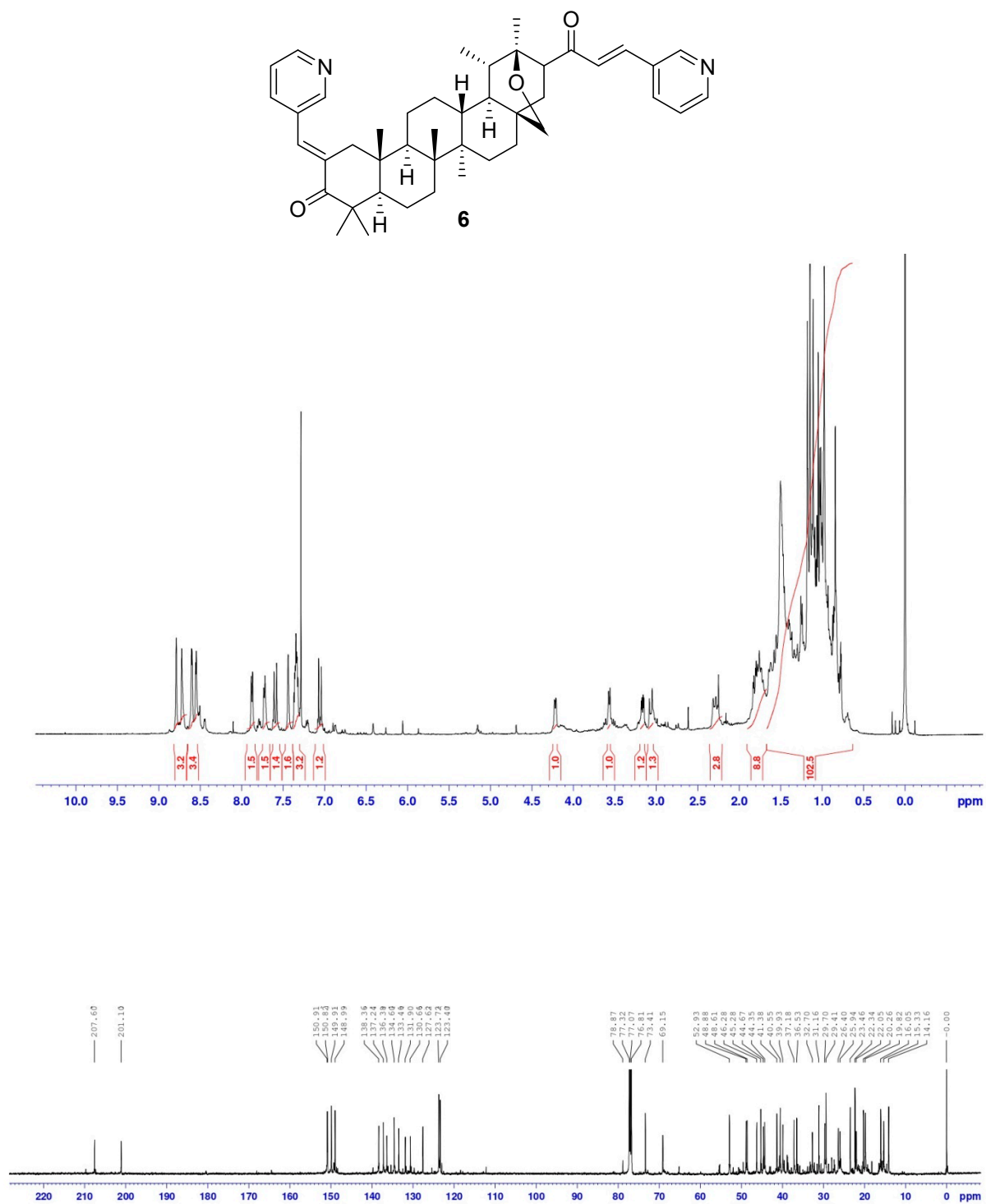


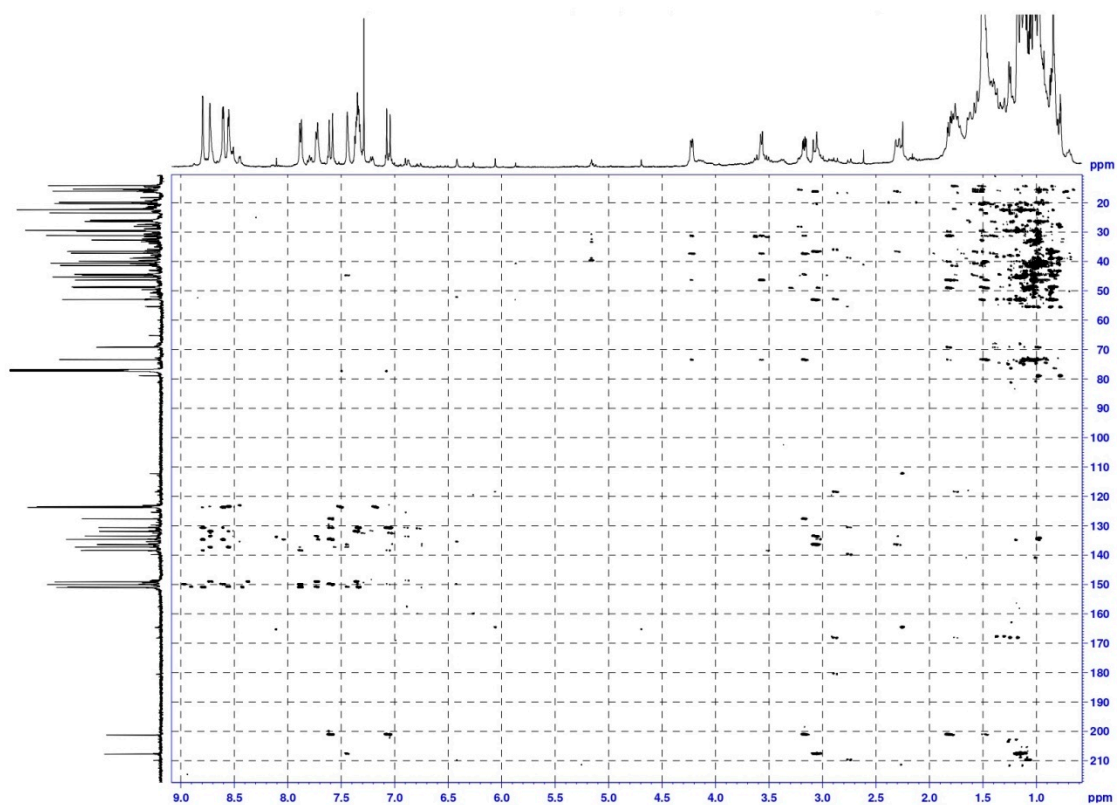
NOESY spectrum of compound 4

**Figure S2.** NMR spectra of compound **5**

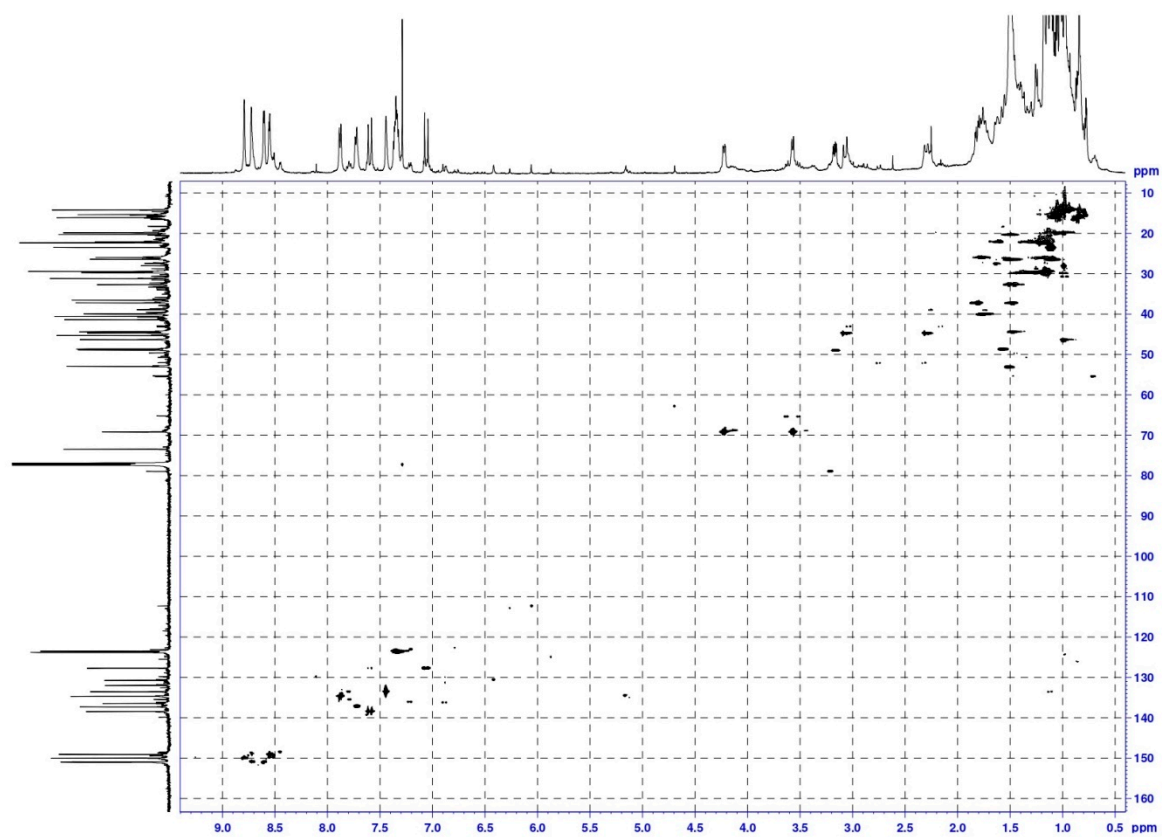


**Figure S3.** NMR spectra of compound **6**

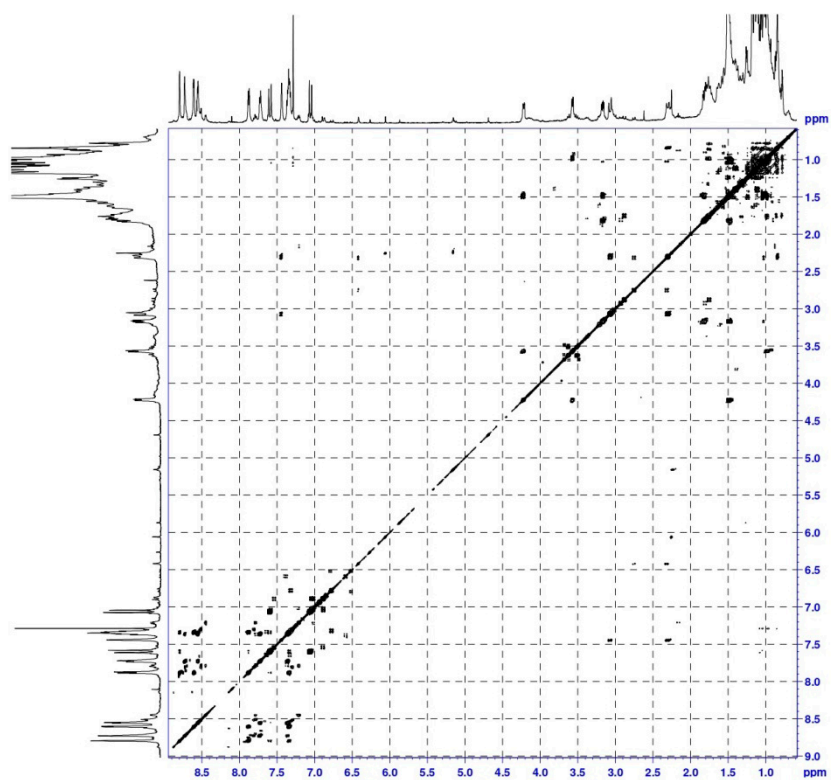




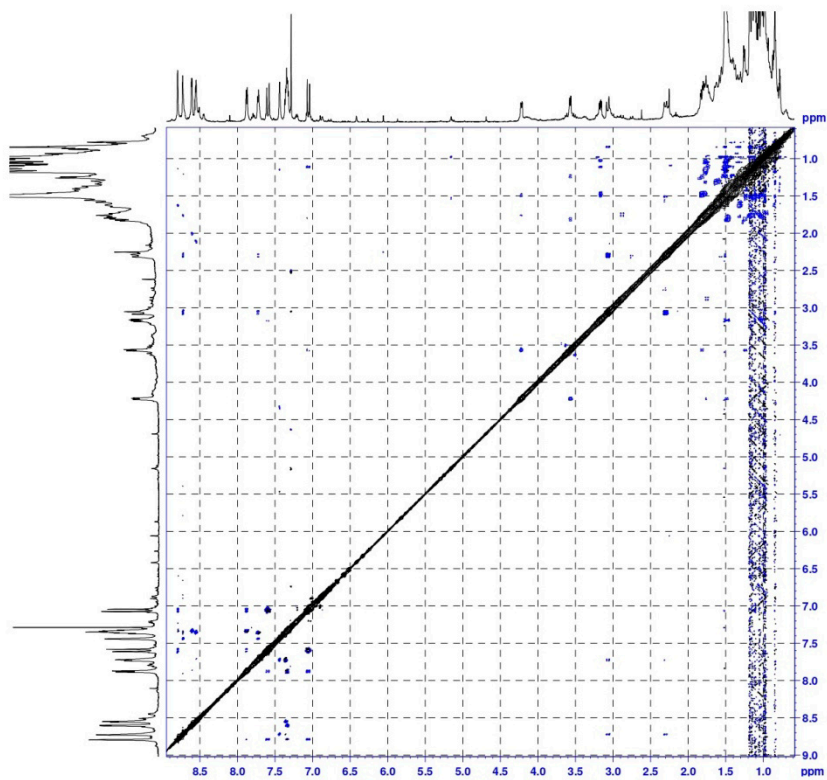
HMBC spectrum of compound 6



HSQC spectrum of compound 6

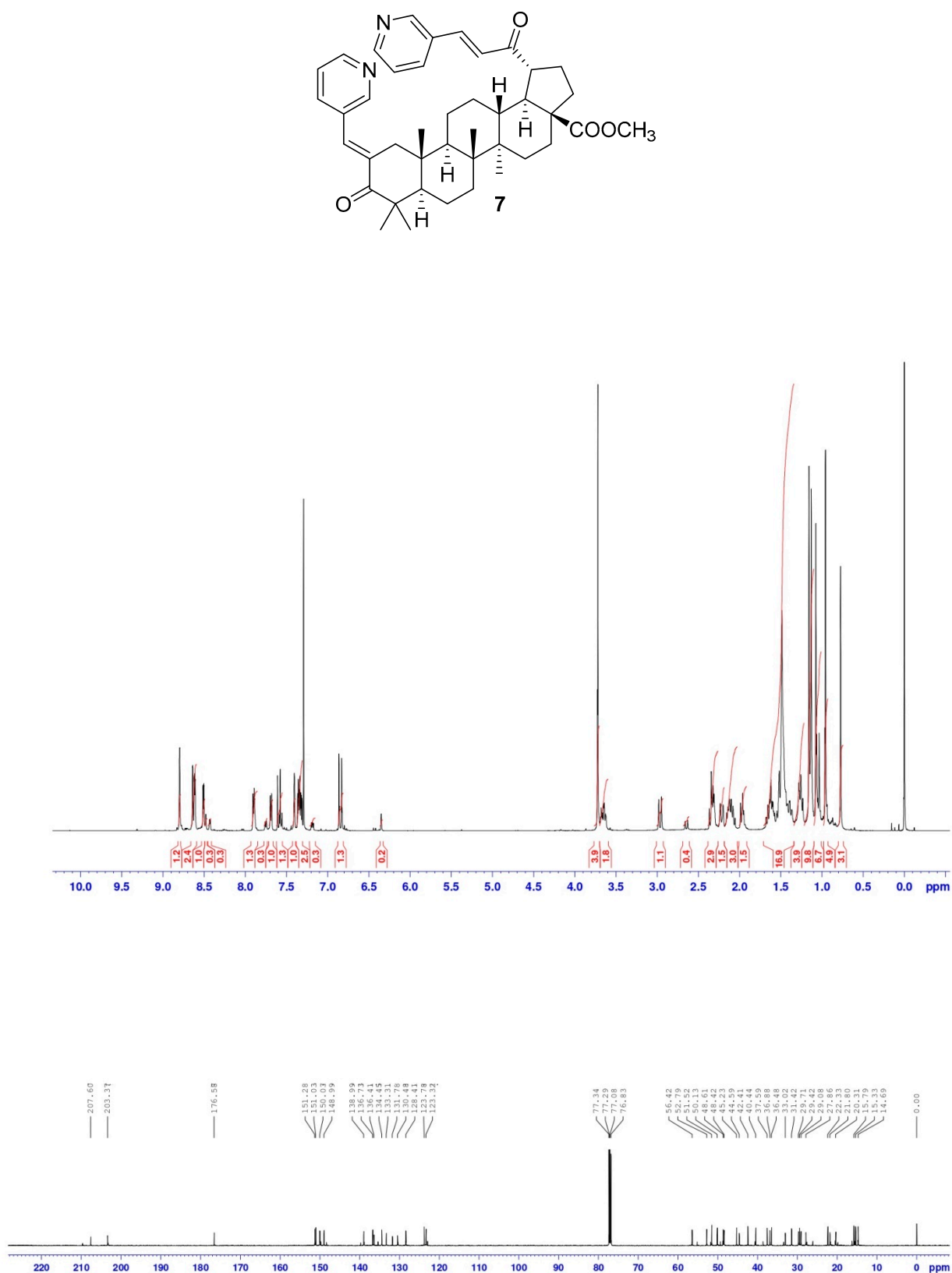


COSY spectrum of compound **6**

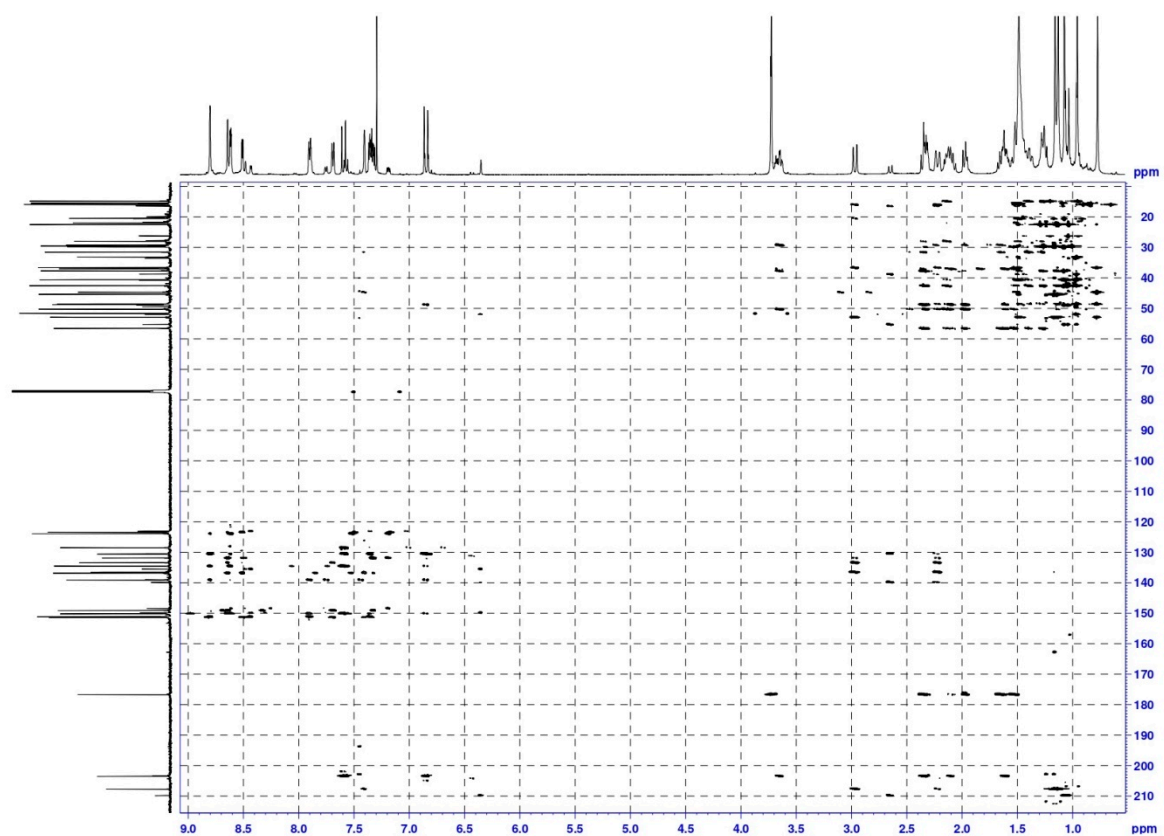


NOESY spectrum of compound **6**

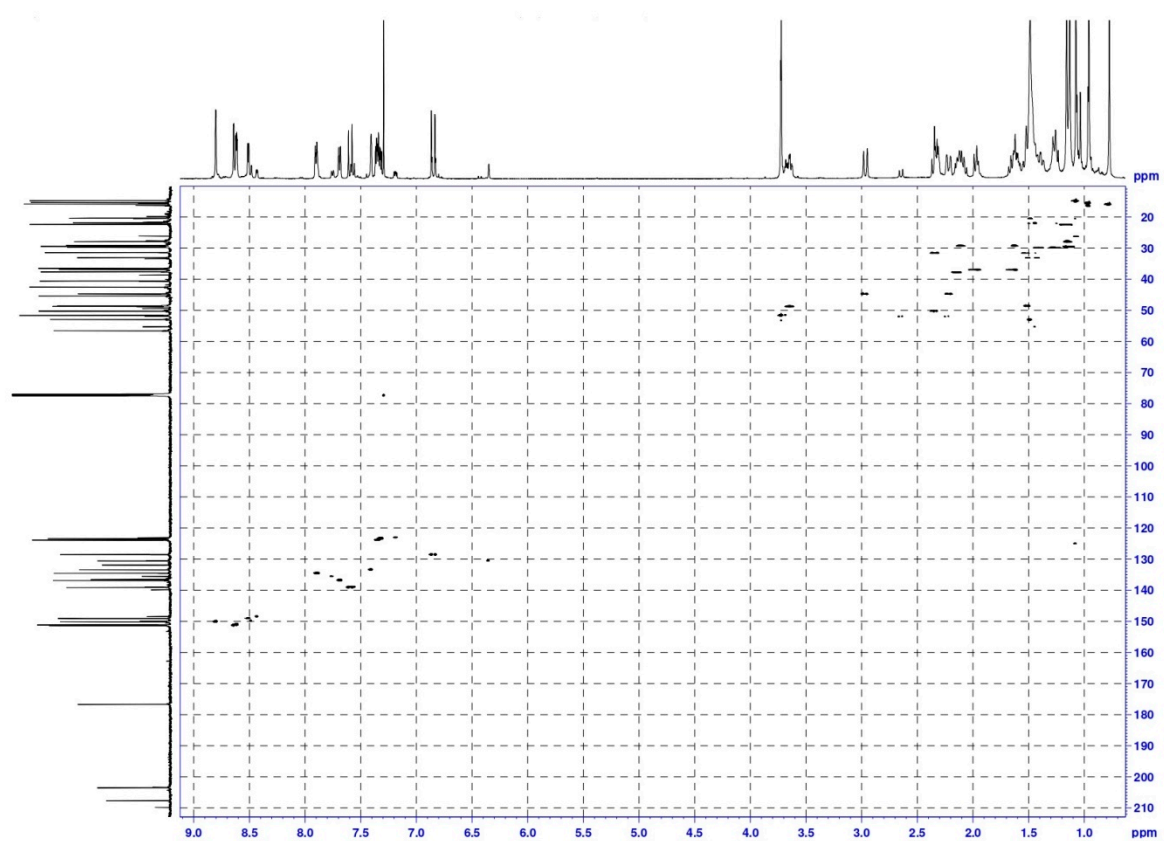
**Figure S4.** NMR spectra of compound **7**



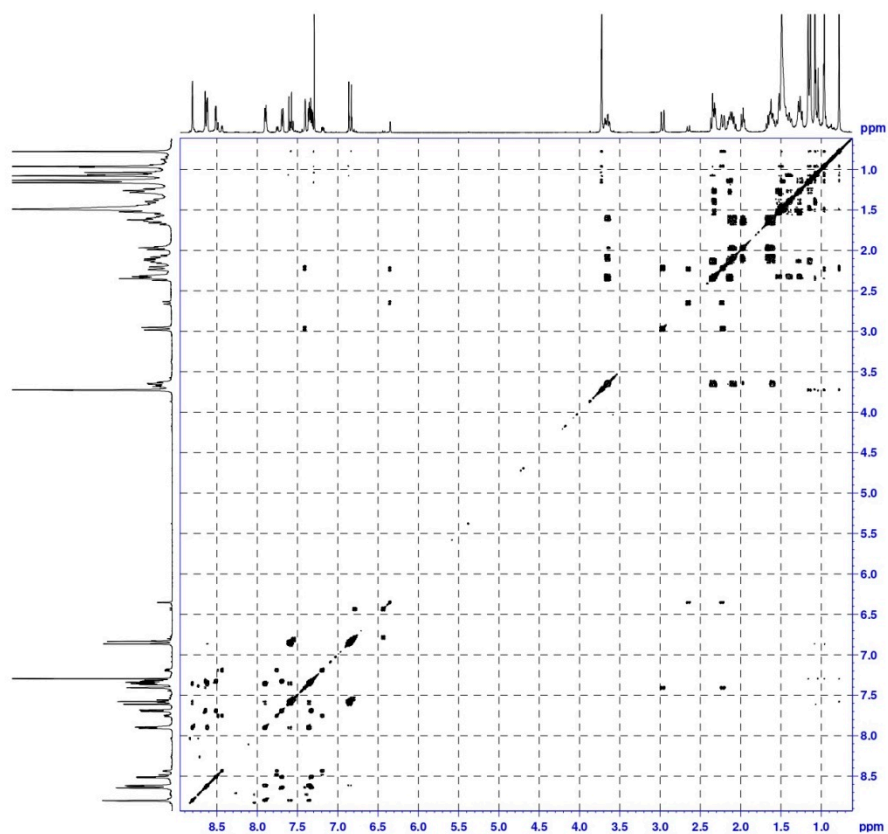




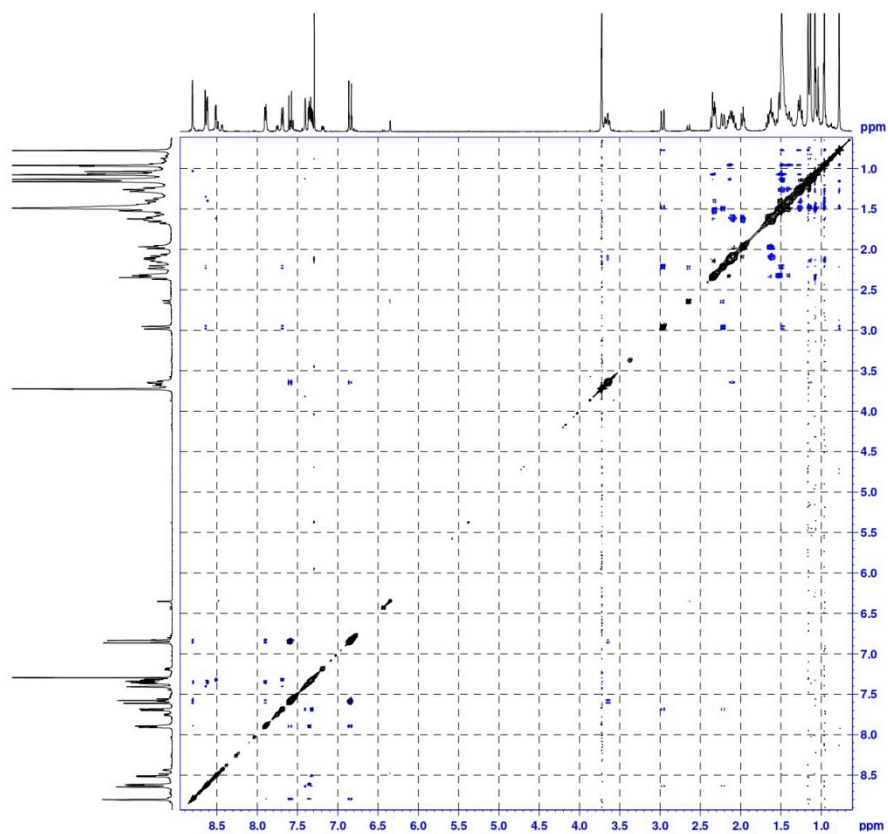
HMBC spectrum of compound **7**



HSQC spectrum of compound **7**



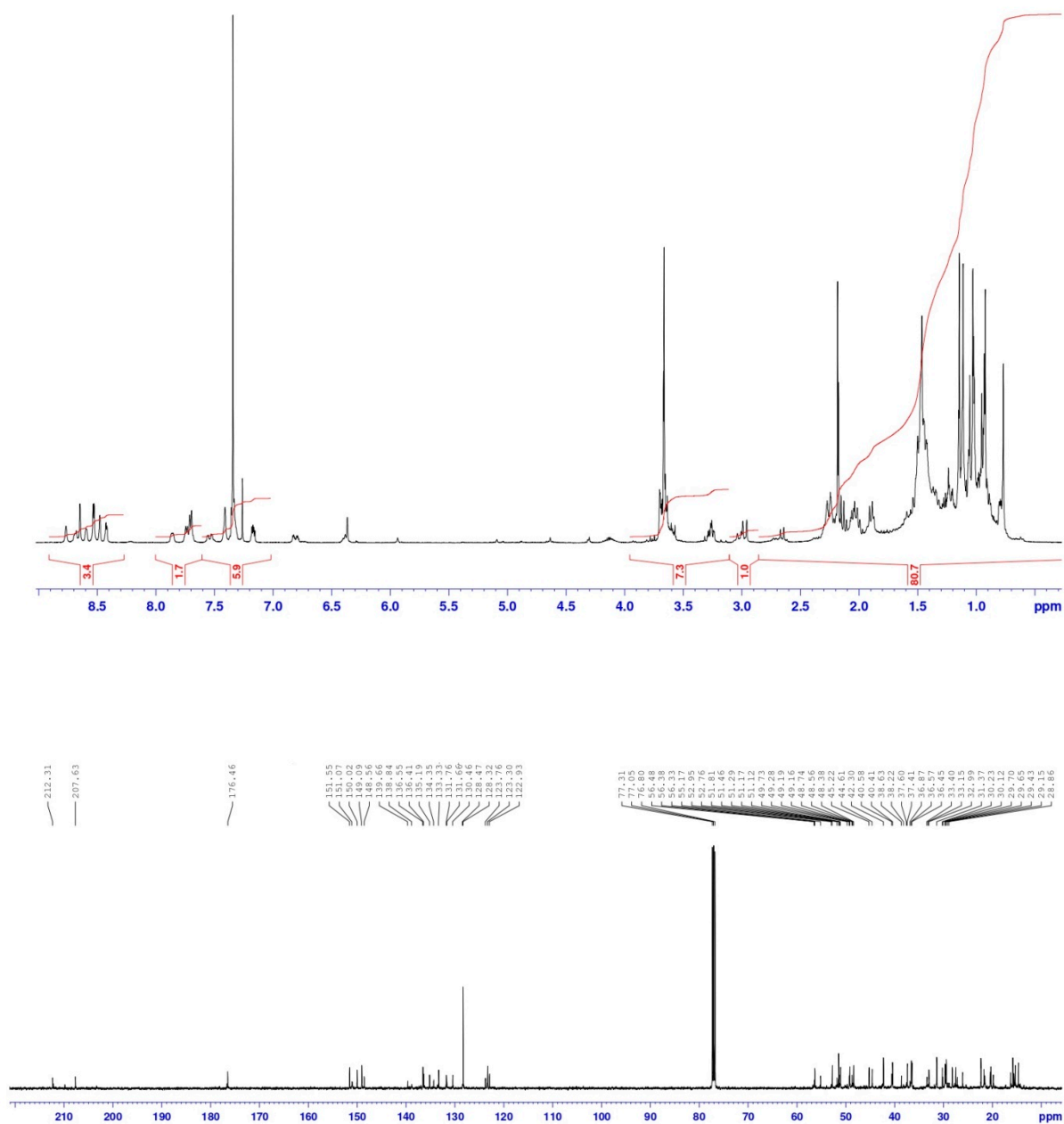
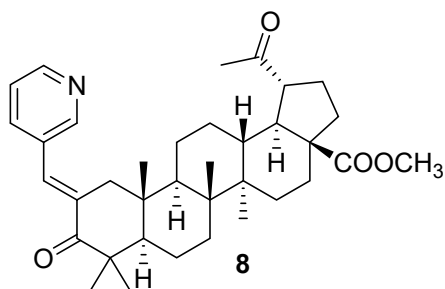
COSY spectrum of compound 7



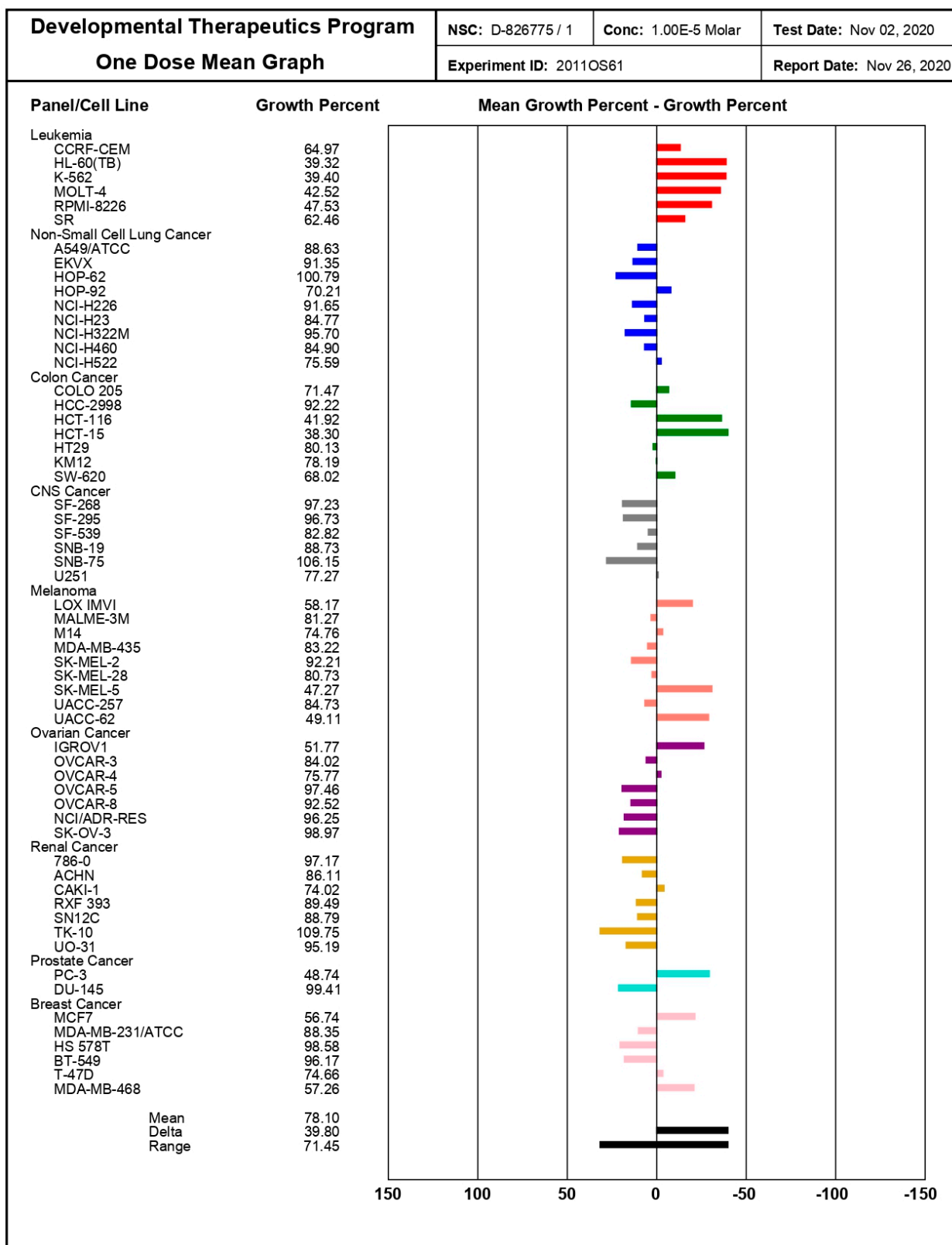
NOESY spectrum of compound 7



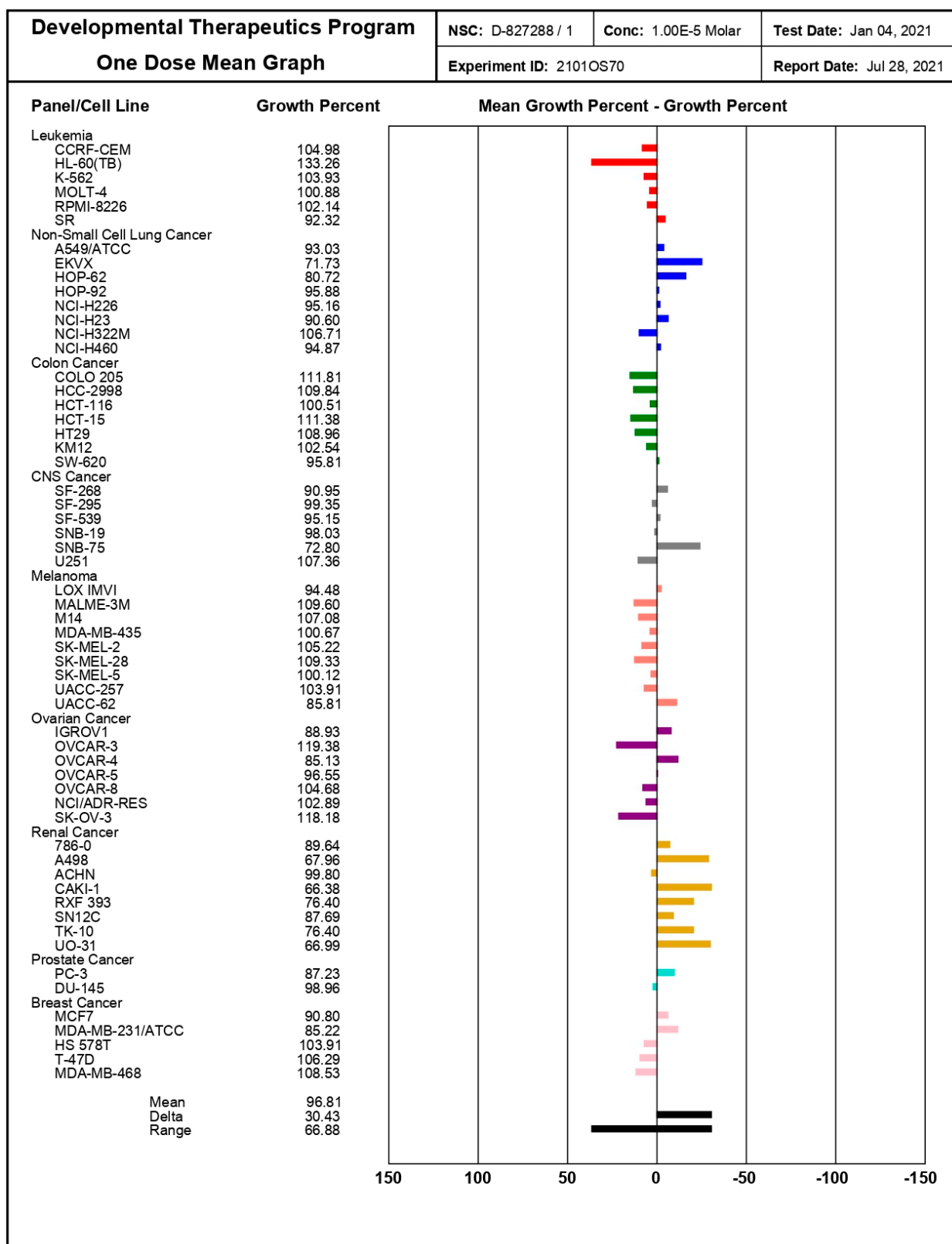
**Figure S5.** NMR spectra of compound **8**



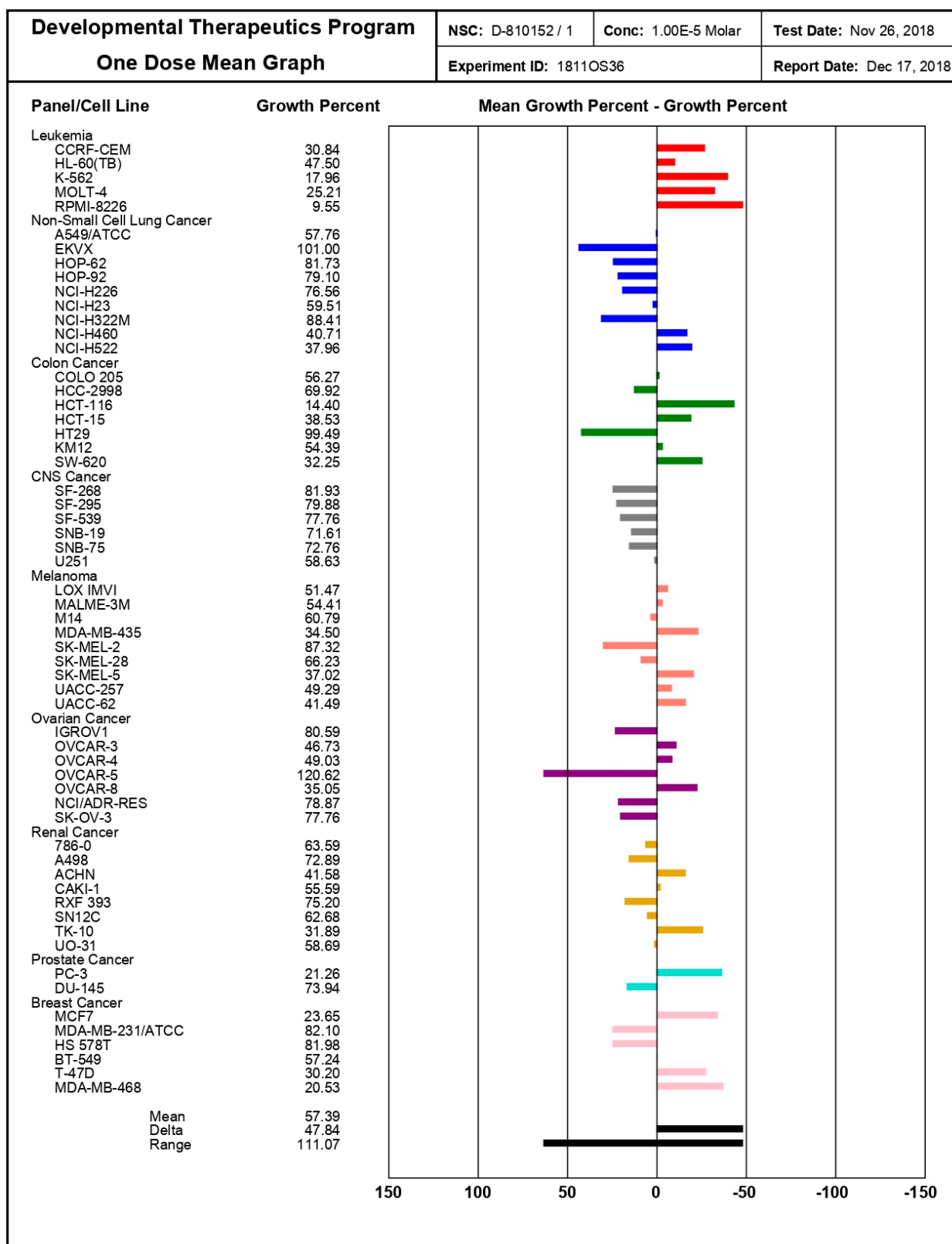
**Figure S6.** *In vitro* antitumor activity of compound **1** against human cancer cells of 60 lines at a concentration of 100  $\mu$ M



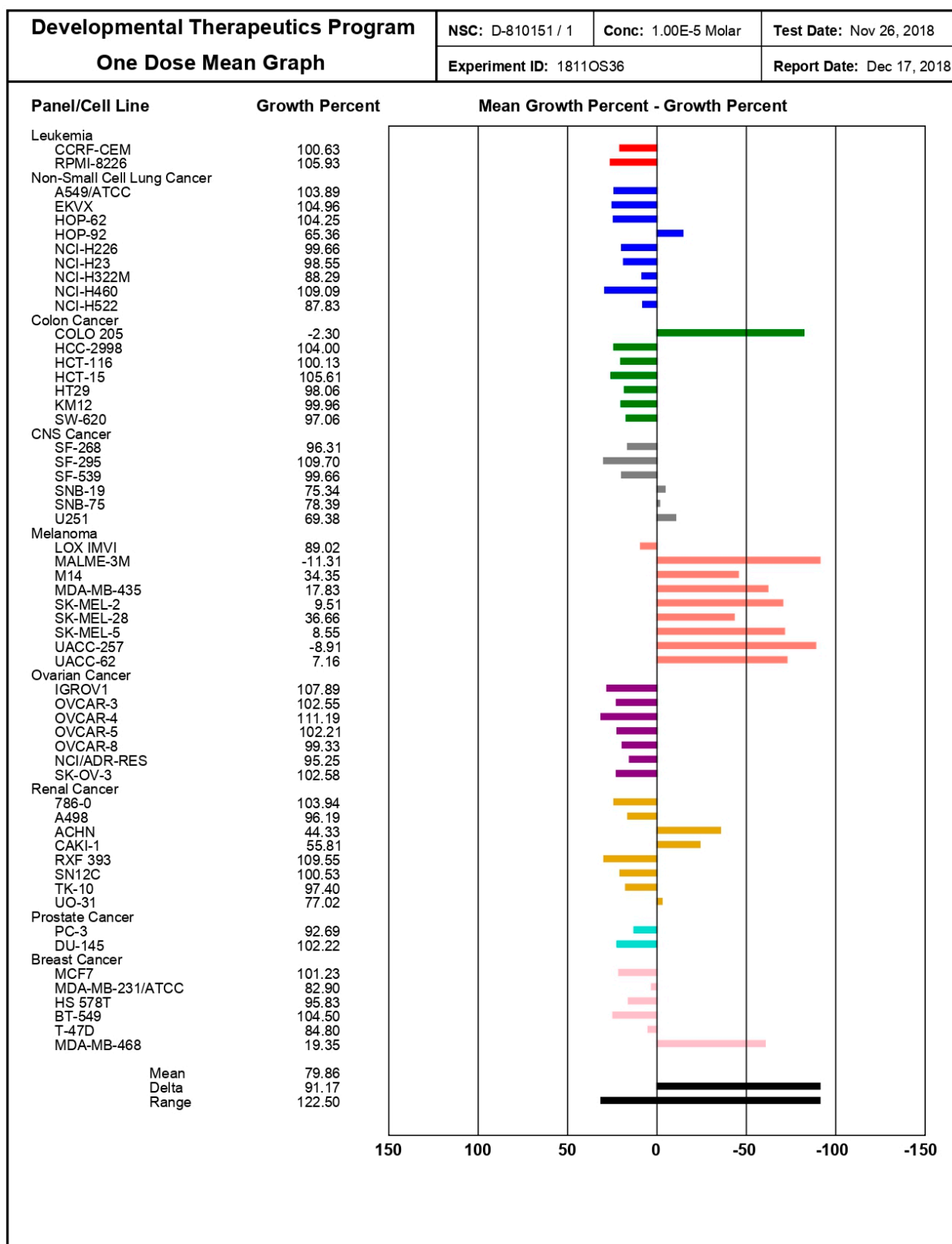
**Figure S7.** *In vitro* antitumor activity of compound **2** against human cancer cells of 60 lines at a concentration of 100  $\mu$ M



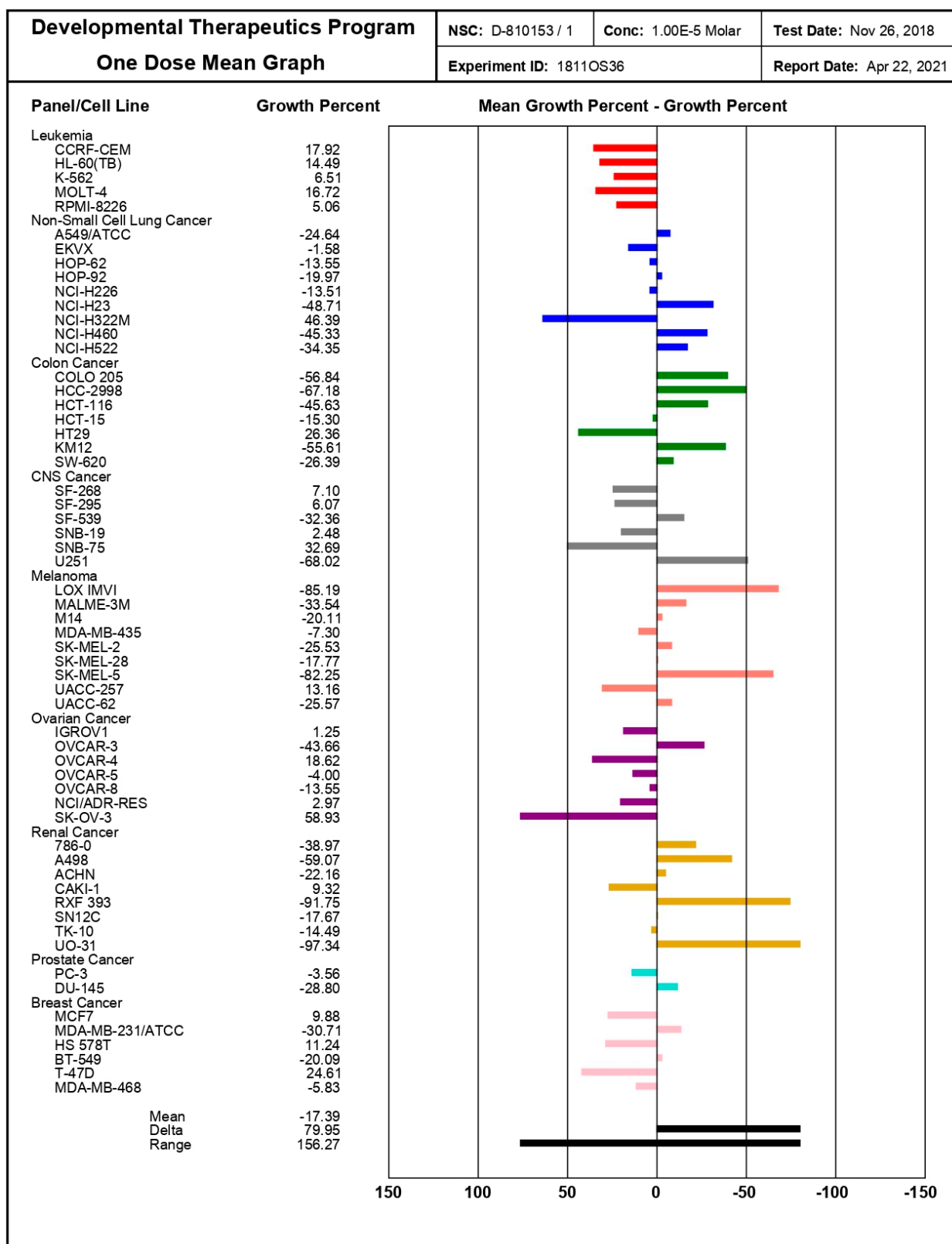
**Figure S8.** *In vitro* antitumor activity of compound **4** against human cancer cells of 60 lines at a concentration of 100  $\mu$ M



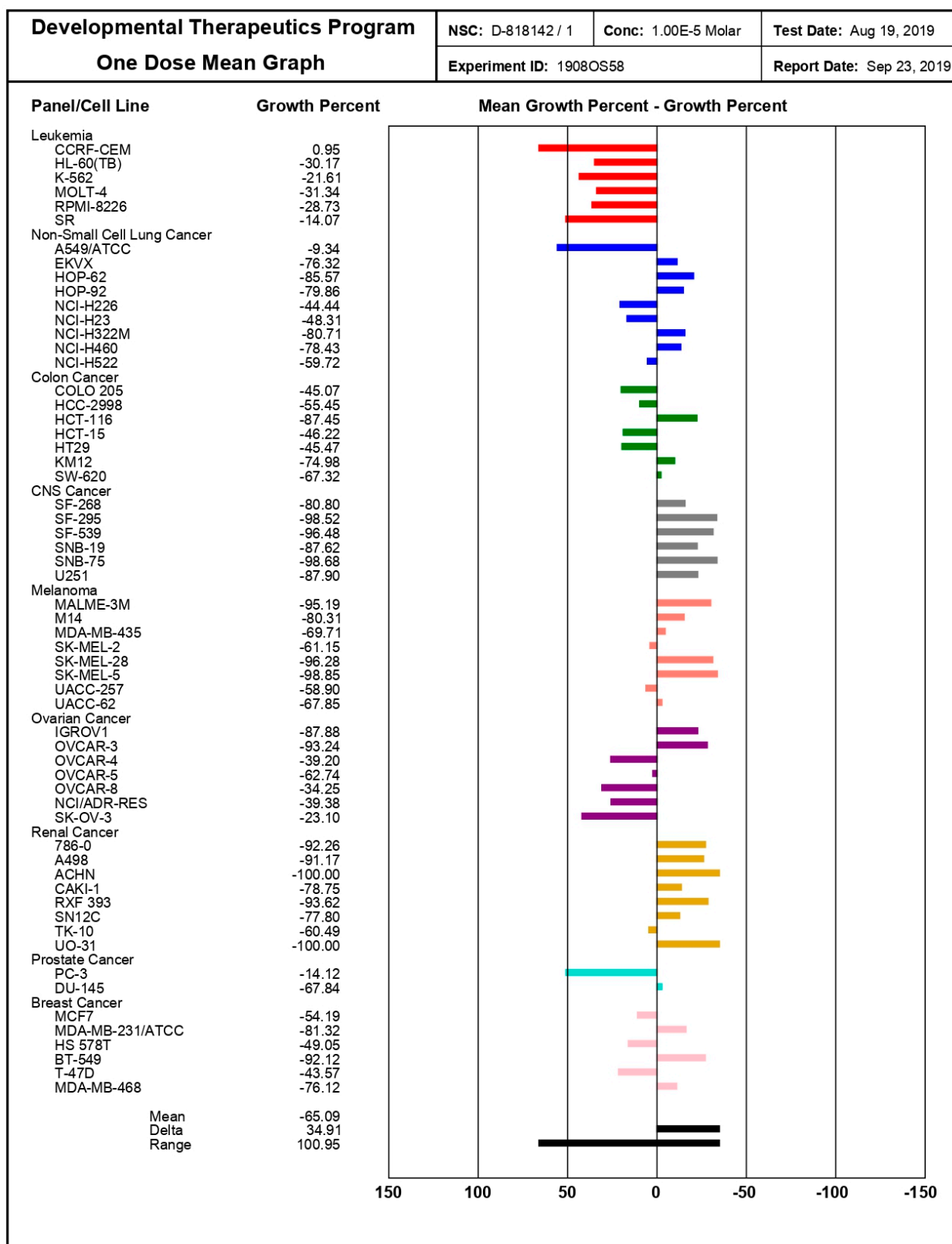
**Figure S9.** *In vitro* antitumor activity of compound **5** against human cancer cells of 60 lines at a concentration of 100  $\mu$ M



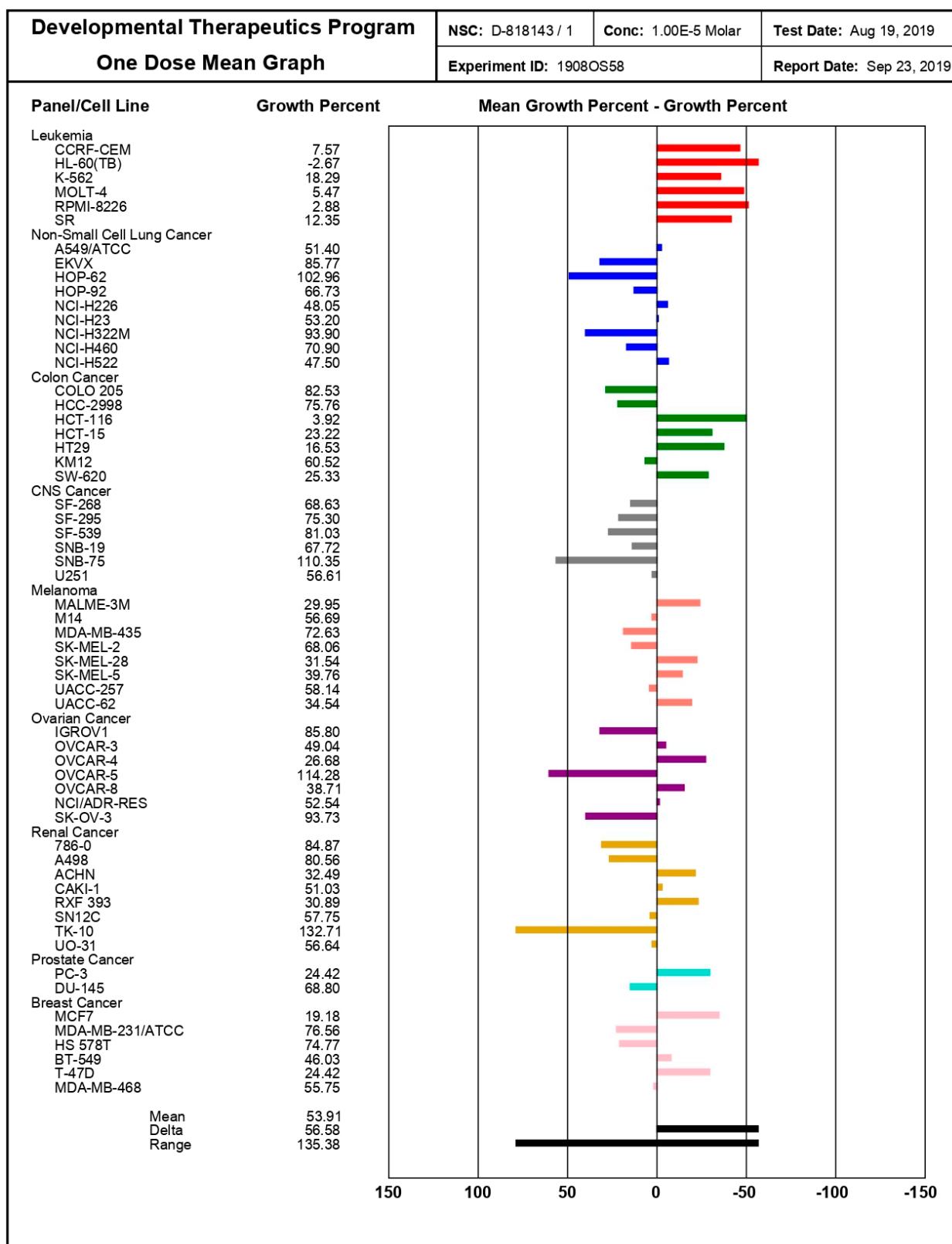
**Figure S10.** *In vitro* antitumor activity of compound **6** against human cancer cells of 60 lines at a concentration of 100  $\mu$ M



**Figure S11.** *In vitro* antitumor activity of compound **7** against human cancer cells of 60 lines at a concentration of 100  $\mu$ M

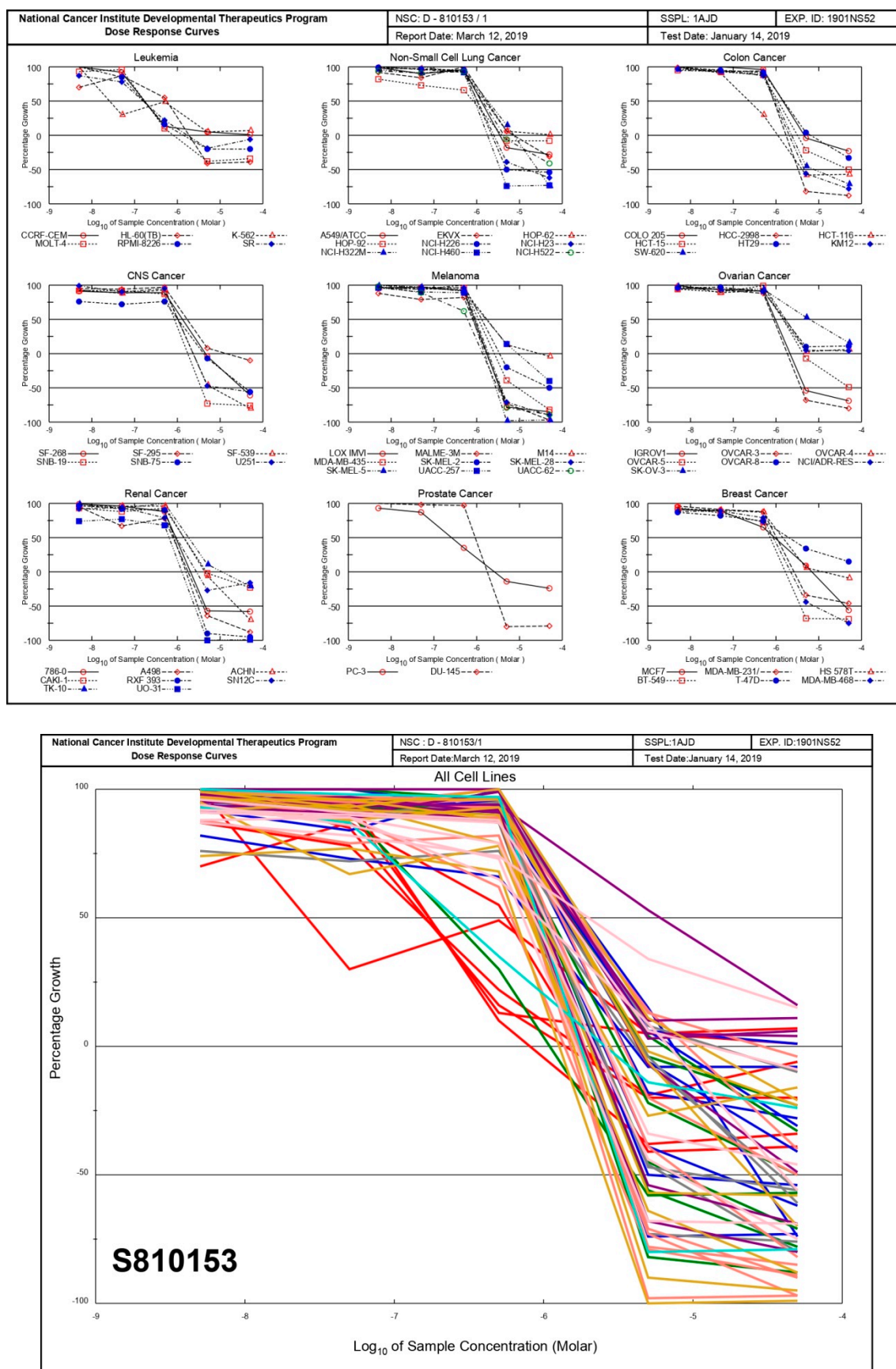


**Figure S12.** *In vitro* antitumor activity of compound **8** against human cancer cells of 60 lines at a concentration of 100  $\mu$ M



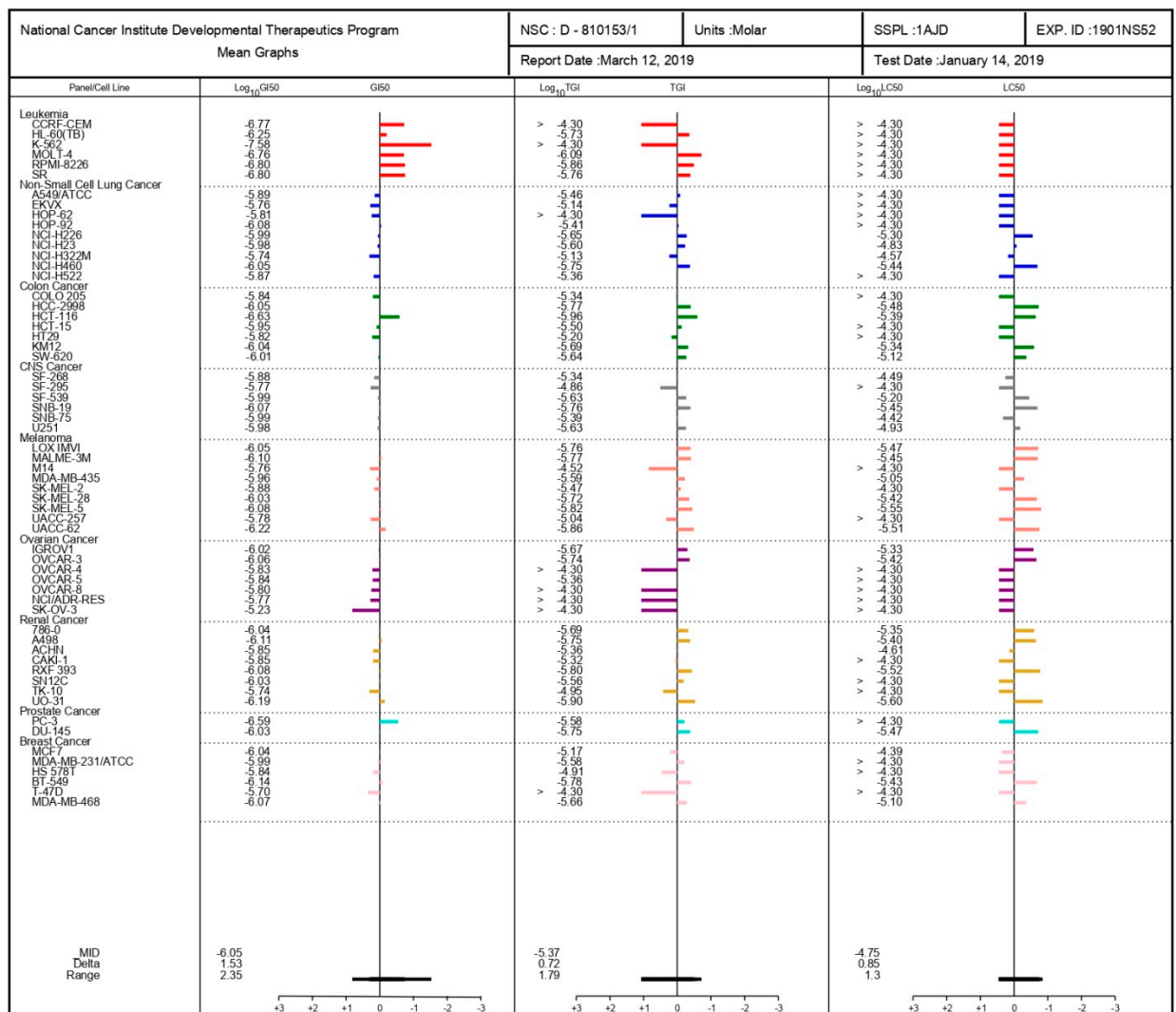


**Figure S13.** *In vitro* anticancer activity of compound **6** against 60 human cancer cell lines in concentrations 0.01 – 100  $\mu$ M

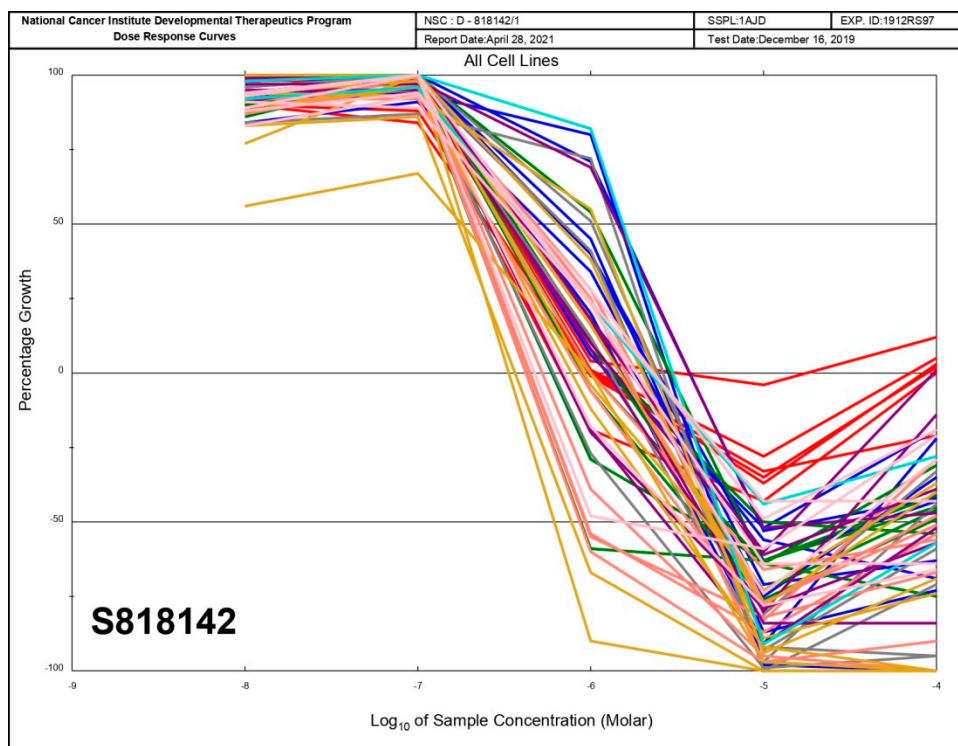
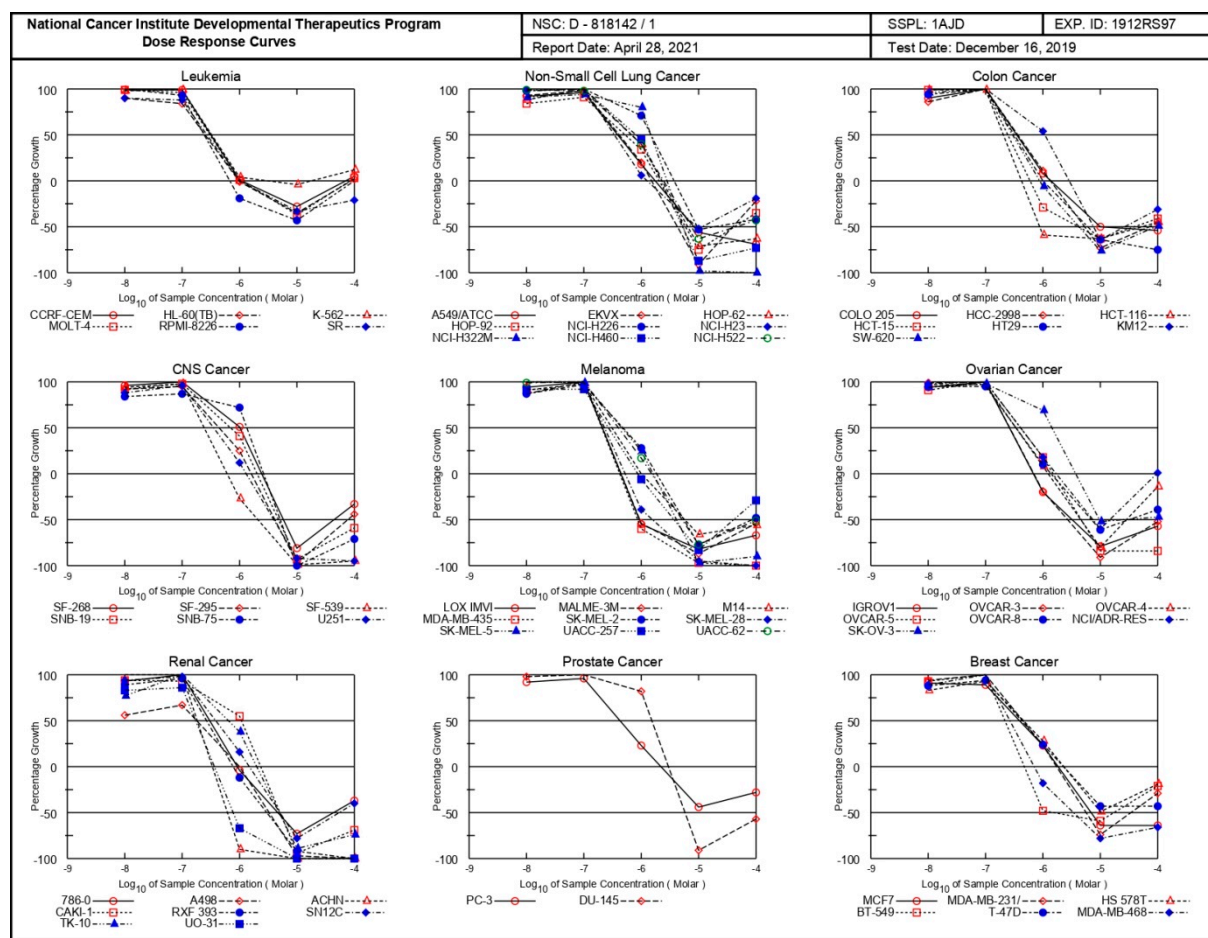


**National Cancer Institute Developmental Therapeutics Program  
In-Vitro Testing Results**

NSC : D - 810153 / 1				Experiment ID : 1901NS52								Test Type : 08				Units : Molar	
Report Date : March 12, 2019				Test Date : January 14, 2019								QNS :				MC :	
COMI : 3-oxo-F-2sr-3NK				Stain Reagent : SRB Dual-Pass Related								SSPL : 1AJD					
Log10 Concentration																	
Panel/Cell Line	Time Zero	Ctrl	-8.3	-7.3	-6.3	-5.3	-4.3	-8.3	-7.3	-6.3	-5.3	-4.3	GI50	TGI	LC50		
Leukemia																	
CCRF-CEM	0.437	2.443	2.467	2.275	0.696	0.535	0.466	101	92	13	5	1	1.69E-7	> 5.00E-5	> 5.00E-5		
HL-60(TB)	0.908	2.684	2.159	2.449	1.880	0.538	0.550	70	87	55	-41	-39	5.60E-7	1.87E-6	> 5.00E-5		
K-562	0.163	1.581	1.618	0.585	0.855	0.228	0.258	103	30	49	5	7	2.64E-8	> 5.00E-5	> 5.00E-5		
MOLT-4	0.709	2.732	2.595	2.652	0.917	0.443	0.471	93	96	10	-38	-34	1.72E-7	8.21E-7	> 5.00E-5		
RPMI-8226	0.901	2.675	2.681	2.405	1.182	0.718	0.719	100	85	16	-20	-20	1.60E-7	1.37E-6	> 5.00E-5		
SR	0.448	1.554	1.415	1.308	0.696	0.364	0.420	87	78	22	-19	-6	1.58E-7	1.75E-6	> 5.00E-5		
Non-Small Cell Lung Cancer																	
A549/ATCC	0.420	2.203	2.185	2.018	2.136	0.346	0.303	99	90	96	-18	-28	1.27E-6	3.50E-6	> 5.00E-5		
EKVX	0.753	1.663	1.587	1.521	1.669	0.810	0.518	92	84	101	6	-31	1.72E-6	7.32E-6	> 5.00E-5		
HOP-62	0.758	2.664	2.624	2.605	2.530	0.874	0.784	98	97	93	6	1	1.56E-6	> 5.00E-5	> 5.00E-5		
HOP-92	1.219	2.045	1.895	1.820	1.764	1.125	1.127	82	73	66	-8	-8	8.23E-7	3.92E-6	> 5.00E-5		
NCI-H226	1.223	2.808	2.798	2.756	2.722	0.607	0.557	99	97	95	-50	-54	1.02E-6	2.25E-6	4.97E-6		
NCI-H23	0.599	2.141	2.144	2.079	2.015	0.363	0.230	100	96	92	-39	-62	1.04E-6	2.50E-6	1.49E-5		
NCI-H322M	0.663	1.933	1.884	1.816	1.864	0.857	0.171	96	91	95	15	-74	1.82E-6	7.41E-6	2.68E-5		
NCI-H460	0.429	2.805	2.848	2.825	2.613	0.113	0.115	102	101	92	-74	-73	8.95E-7	1.79E-6	3.59E-6		
NCI-H522	0.888	2.628	2.522	2.469	2.503	0.839	0.520	94	91	93	-6	-41	1.36E-6	4.39E-6	> 5.00E-5		
Colon Cancer																	
COLO 205	0.484	2.048	2.098	2.068	1.983	0.463	0.371	103	101	96	-4	-23	1.43E-6	4.53E-6	> 5.00E-5		
HCC-2998	0.731	2.671	2.654	2.537	2.560	0.133	0.089	99	93	94	-82	-88	8.92E-7	1.72E-6	3.30E-6		
HCT-116	0.236	2.490	2.496	2.289	0.903	0.099	0.102	100	91	30	-58	-57	2.33E-7	1.09E-6	4.05E-6		
HCT-15	0.249	1.679	1.611	1.578	1.508	0.195	0.126	95	93	88	-22	-50	1.11E-6	3.17E-6	> 5.00E-5		
HT29	0.259	1.856	1.873	1.777	1.732	0.320	0.174	101	95	92	4	-33	1.50E-6	6.34E-6	> 5.00E-5		
KM12	0.581	2.749	2.686	2.648	2.477	0.256	0.126	97	95	87	-56	-78	9.12E-7	2.03E-6	4.54E-6		
SW-620	0.450	1.863	1.800	1.758	1.716	0.247	0.130	96	93	90	-45	-71	9.84E-7	2.31E-6	7.65E-6		
CNS Cancer																	
SF-268	0.949	2.458	2.327	2.294	2.287	0.911	0.372	91	89	89	-4	-61	1.31E-6	4.53E-6	3.23E-5		
SF-295	0.933	3.000	2.907	2.872	2.947	1.089	0.842	95	94	97	8	-10	1.69E-6	1.37E-5	> 5.00E-5		
SF-539	0.585	2.121	2.012	1.943	2.019	0.313	0.115	93	88	93	-46	-80	1.02E-6	2.33E-6	6.34E-6		
SNB-19	0.780	2.517	2.370	2.374	2.295	0.208	0.185	92	92	87	-73	-76	8.53E-7	1.75E-6	3.58E-6		
SNB-75	1.190	2.041	1.839	1.803	1.835	1.105	0.527	76	72	76	-7	-56	1.02E-6	4.10E-6	3.81E-5		
U251	0.361	1.860	1.843	1.717	1.791	0.193	0.159	99	90	95	-47	-56	1.04E-6	2.35E-6	1.17E-5		
Melanoma																	
LOX IMVI	0.445	2.927	2.837	2.841	2.733	0.098	0.066	96	97	92	-78	-85	8.85E-7	1.74E-6	3.42E-6		
MALME-3M	0.876	1.979	1.842	1.743	1.777	0.233	0.024	88	79	82	-73	-97	8.00E-7	1.68E-6	3.53E-6		
M14	0.547	2.493	2.408	2.401	2.366	0.808	0.526	96	95	93	13	-4	1.74E-6	2.99E-5	> 5.00E-5		
MDA-MB-435	0.766	2.919	2.848	2.795	2.825	0.467	0.137	97	94	96	-39	-82	1.09E-6	2.57E-6	8.98E-6		
SK-MEL-2	1.055	2.781	2.719	2.675	2.785	0.841	0.527	96	94	100	-20	-50	1.30E-6	3.39E-6	4.98E-5		
SK-MEL-28	0.812	2.498	2.505	2.450	2.429	0.240	0.085	100	97	96	-71	-90	9.44E-7	1.88E-6	3.76E-6		
SK-MEL-5	0.982	3.242	3.221	3.181	3.036	0.024	0.029	99	97	91	-98	-97	8.24E-7	1.52E-6	2.80E-6		
UACC-257	1.152	2.628	2.566	2.484	2.471	1.364	0.689	96	90	89	14	-40	1.67E-6	9.16E-6	> 5.00E-5		
UACC-62	1.153	3.010	2.968	2.813	2.296	0.246	0.125	98	89	62	-79	-89	6.04E-7	1.37E-6	3.12E-6		
Ovarian Cancer																	
IGROV1	0.550	2.231	2.141	2.127	2.079	0.254	0.169	95	94	91	-54	-69	9.59E-7	2.12E-6	4.71E-6		
OVCAR-3	0.634	2.100	2.080	1.991	1.929	0.203	0.127	99	93	88	-68	-80	8.79E-7	1.84E-6	3.84E-6		
OVCAR-4	0.694	1.533	1.536	1.444	1.468	0.718	0.747	100	89	92	3	6	1.49E-6	> 5.00E-5	> 5.00E-5		
OVCAR-5	0.617	1.777	1.711	1.658	1.769	0.576	0.316	94	90	99	-7	-49	1.46E-6	4.32E-6	> 5.00E-5		
OVCAR-8	0.474	2.182	2.112	2.133	2.035	0.638	0.664	96	97	91	10	11	1.60E-6	> 5.00E-5	> 5.00E-5		
NCI/ADR-RES	0.543	1.864	1.876	1.860	1.881	0.608	0.602	101	100	101	5	4	1.70E-6	> 5.00E-5	> 5.00E-5		
SK-OV-3	0.914	2.247	2.217	2.171	2.166	1.616	1.126	98	94	94	53	16	5.90E-6	> 5.00E-5	> 5.00E-5		
Renal Cancer																	
786-0	0.836	2.935	2.923	2.848	2.682	0.362	0.351	99	96	88	-57	-58	9.15E-7	2.03E-6	4.49E-6		
A498	2.033	2.648	2.619	2.447	2.511	0.726	0.240	95	67	78	-64	-88	7.83E-7	1.76E-6	3.97E-6		
ACHN	0.450	1.967	1.913	1.908	1.907	0.424	0.136	96	96	96	-6	-70	1.41E-6	4.38E-6	2.44E-5		
CAKI-1	0.880	2.478	2.368	2.287	2.369	0.863	0.676	93	88	93	-2	-23	1.42E-6	4.77E-6	> 5.00E-5		
RXF 393	0.904	1.517	1.501	1.468	1.456	0.090	0.048	97	92	90	-90	-95	8.34E-7	1.58E-6	2.99E-6		
SN12C	0.660	2.827	2.660	2.688	2.368	0.481	0.552	92	94	79	-27	-16	9.35E-7	2.77E-6	> 5.00E-5		
TK-10	0.576	2.044	2.031	1.941	2.042	0.744	0.455	99	93	100	11	-21	1.83E-6	1.12E-5	> 5.00E-5		
UO-31	1.055	2.370	2.026	2.065	1.952		0.008	74	77	68	-100	-99	6.41E-7	1.27E-6	2.52E-6		
Prostate Cancer																	
PC-3	0.610	2.557	2.411	2.300	1.286	0.528	0.462	93	87	35	-14	-24	2.55E-7	2.62E-6	> 5.00E-5		
DU-145	0.500	2.020	2.099	1.994	1.980	0.101	0.106	105	98	97	-80	-79	9.25E-7	1.77E-6	3.39E-6		
Breast Cancer																	
MCF7	0.494	2.442	2.274	2.226	1.752	0.665	0.219	91	89	65	9	-56	9.12E-7	6.84E-6	4.08E-5		
MDA-MB-231/ATCC	0.676	1.663	1.624	1.574	1.544	0.449	0.367	96	91	88	-34	-46	1.03E-6	2.64E-6	> 5.00E-5		
HS 578T	1.244	2.193	2.115	2.099	2.072	1.302	1.129	92	90	87	6	-9	1.44E-6	1.24E-5	> 5.00E-5		
BT-549	1.117	2.299	2.226	2.132	1.984	0.360	0.344	94	86	73	-68	-69	7.32E-7	1.65E-6	3.74E-6		
T-47D	0.804	2.255	2.063	1.999	1.880	1.294	1.026	87	82	74	34	15	1.98E-6	> 5.00E-5	> 5.00E-5		
MDA-MB-468	0.998	1.613	1.538	1.545	1.483	0.560	0.253	88	89	79	-44	-75	8.59E-7	2.19E-6	7.87E-6		



**Figure S14.** *In vitro* anticancer activity of compound **7** against 60 human cancer cell lines in concentrations 0.01 – 100  $\mu$ M



# National Cancer Institute Developmental Therapeutics Program In-Vitro Testing Results

NSC : D - 818142 / 1			Experiment ID : 1912RS97										Test Type : 08		Units : Molar	
Report Date : April 28, 2021			Test Date : December 16, 2019										QNS :		MC :	
COMI : OMeBk-2,30-3NK			Stain Reagent : SRB Dual-Pass Related										SSPL : 1AJD			
Log10 Concentration																
Panel/Cell Line	Time 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	0.487	3.148	3.131	3.111	0.506	0.351	0.627	99	99	1	-28	5	3.14E-7		> 1.00E-4	
HL-60(TB)	0.406	2.016	1.850	1.752	0.401	0.262	0.432	90	84	-1	-35	2	2.48E-7		> 1.00E-4	
K-562	0.188	2.259	2.216	2.245	0.264	0.180	0.434	98	99	4	-4	12	3.28E-7		> 1.00E-4	
MOLT-4	0.547	2.729	2.710	2.647	0.558	0.346	0.619	99	96	1	-37	3	3.04E-7		> 1.00E-4	
RPMI-8226	0.785	3.076	3.082	2.907	0.639	0.447	0.781	100	93	-19	-43		2.42E-7	6.80E-7	> 1.00E-4	
SR	0.274	1.575	1.441	1.413	0.272	0.183	0.218	90	88		-33	-21	2.66E-7	9.81E-7	> 1.00E-4	
Non-Small Cell Lung Cancer																
A549/ATCC	0.451	2.512	2.349	2.424	0.816	0.201	0.142	92	96	18	-56	-69	3.85E-7	1.74E-6	8.40E-6	
EKVX	0.739	2.179	2.073	2.157	1.021	0.065	0.575	93	98	20	-91	-22	4.12E-7	1.50E-6		
HOP-62	0.765	2.739	2.505	2.796	1.551	0.220	0.282	88	103	40	-71	-63	6.89E-7	2.28E-6	6.44E-6	
HOP-92	1.240	2.019	1.892	1.946	1.507	0.307	0.801	84	91	34	-75	-35	5.26E-7	2.06E-6		
NCI-H226	0.851	1.506	1.496	1.552	1.316	0.404	0.495	98	107	71	-53	-42	1.48E-6	3.76E-6		
NCI-H23	0.613	2.131	2.105	2.156	0.700	0.297	0.499	98	102	6	-52	-19	3.46E-7	1.26E-6		
NCI-H322M	0.736	2.174	2.051	2.095	1.888	0.017	-0.100	91	94	80	-98	-100	1.48E-6	2.82E-6	5.39E-6	
NCI-H460	0.403	3.227	3.239	3.248	1.686	0.053	0.108	100	101	45	-87	-73	8.27E-7	2.20E-6	5.26E-6	
NCI-H522	1.646	3.270	3.251	3.231	2.289	0.610	0.941	99	98	40	-63	-43	6.61E-7	2.43E-6		
Colon Cancer																
COLO 205	0.438	2.051	1.886	2.088	0.561	0.219	0.202	90	102	8	-50	-54	3.57E-7	1.35E-6	9.95E-6	
HCC-2998	0.812	2.701	2.427	2.713	1.023	0.218	0.441	86	101	11	-73	-46	3.68E-7	1.36E-6		
HCT-116	0.279	2.470	2.439	2.447	0.114	0.104	0.154	99	99	-59	-63	-45	2.04E-7	4.23E-7		
HCT-15	0.280	1.661	1.649	1.661	0.199	0.104	0.166	99	100	-29	-63	-41	2.44E-7	5.96E-7		
HT29	0.402	2.535	2.417	2.543	0.411	0.143	0.102	94	100		-64	-75	3.19E-7	1.02E-6	5.99E-6	
KM12	0.607	3.127	3.136	3.120	1.961	0.216	0.420	100	100	54	-64	-31	1.08E-6	2.85E-6		
SW-620	0.319	2.556	2.469	2.588	0.299	0.076	0.164	96	101	-6	-76	-49	3.00E-7	8.72E-7		
CNS Cancer																
SF-268	0.931	3.000	2.915	3.004	1.981	0.175	0.626	96	100	51	-81	-33	1.01E-6	2.42E-6		
SF-295	0.443	2.244	2.108	2.159	0.887	0.012	0.246	92	95	25	-97	-44	4.37E-7	1.59E-6		
SF-539	0.878	3.028	2.890	2.982	0.641	0.010	0.046	94	98	-27	-99	-95	2.42E-7	6.08E-7	2.09E-6	
SNB-19	0.591	2.211	2.086	2.181	1.250	0.044	0.240	92	98	41	-93	-59	6.88E-7	2.02E-6	4.79E-6	
SNB-75	2.041	3.206	3.016	3.059	2.883	-0.001	0.601	84	87	72	-100	-71	1.35E-6	2.63E-6	5.12E-6	
U251	0.464	2.326	2.110	2.261	0.697	0.035	0.023	88	96	12	-92	-95	3.58E-7	1.32E-6	3.94E-6	
Melanoma																
LOX IMVI	0.303	2.218	2.102	2.216	0.137	0.055	0.099	94	100	-55	-82	-67	2.10E-7	4.42E-7	9.31E-7	
MALME-3M	0.604	1.508	1.388	1.512	0.277	0.079	0.277	87	100	-54	-87	-54	2.12E-7	4.46E-7	9.39E-7	
M14	0.497	2.229	2.077	2.195	0.504	0.170	0.218	91	98		-66	-56	3.10E-7	1.01E-6	5.77E-6	
MDA-MB-435	0.791	3.257	3.249	3.247	0.314	0.024	-0.179	100	100	-60	-97	-100	2.04E-7	4.20E-7	8.62E-7	
SK-MEL-2	1.053	2.088	1.951	2.053	1.339	0.237	0.553	87	97	28	-77	-48	4.73E-7	1.83E-6		
SK-MEL-28	0.642	2.067	2.112	2.141	0.389	0.033	-0.001	103	105	-39	-95	-100	2.41E-7	5.34E-7	1.55E-6	
SK-MEL-5	0.996	3.318	3.307	3.297	1.576	0.029	0.103	100	99	25	-97	-90	4.60E-7	1.60E-6	4.11E-6	
UACC-257	1.150	2.786	2.659	2.663	1.084	0.199	0.811	92	92	-6	-83	-29	2.71E-7	8.74E-7		
UACC-62	0.905	3.029	3.010	3.036	1.268	0.206	0.443	99	100	17	-77	-51	4.02E-7	1.52E-6	5.14E-6	
Ovarian Cancer																
IGROV1	0.436	2.117	2.014	2.145	0.351	0.090	0.187	94	102	-20	-79	-57	2.67E-7	6.89E-7	3.23E-6	
OVCA-3	0.529	1.949	1.929	2.001	0.428	0.045	0.256	99	104	-19	-91	-52	2.74E-7	6.99E-7	2.67E-6	
OVCA-4	0.815	1.905	1.877	1.868	0.902	0.162	0.701	97	97	8	-80	-14	3.35E-7	1.23E-6		
OVCA-5	0.564	1.416	1.342	1.417	0.716	0.091	0.089	91	100	18	-84	-84	4.07E-7	1.50E-6	4.65E-6	
OVCA-8	0.646	2.862	2.754	2.748	0.866	0.249	0.395	95	95	10	-61	-39	3.37E-7	1.38E-6		
NCI/ADR-RES	0.454	1.655	1.632	1.720	0.675	0.181	0.465	98	105	18	-60	1	4.33E-7			
SK-OV-3	0.661	1.905	1.832	1.883	1.516	0.318	0.349	94	98	69	-52	-47	1.43E-6	3.71E-6		
Renal Cancer																
786-0	0.498	2.201	2.077	2.227	0.480	0.132	0.313	93	101	-4	-73	-37	3.09E-7	9.22E-7		
A498	1.944	2.452	2.227	2.287	1.939	0.053	-0.127	56	67		-97	-100	1.81E-7	9.91E-7	3.26E-6	
ACHN	0.301	1.219	1.219	1.264	0.031	-0.012	-0.098	100	105	-90	-100	-100	1.91E-7	3.46E-7	6.25E-7	
CAKI-1	1.105	3.055	2.933	2.922	2.184	0.062	0.343	94	93	55	-94	-69	1.09E-6	2.34E-6	5.05E-6	
RXF-393	1.595	2.466	2.372	2.429	1.402	0.123	-0.068	89	96	-12	-92	-100	2.65E-7	7.72E-7	2.97E-6	
SN12C	0.525	2.341	2.225	2.311	0.821	0.114	0.315	94	98	16	-78	-40	3.88E-7	1.49E-6		
TK-10	1.057	2.018	1.797	2.062	1.418	0.120	0.279	77	104	38	-89	-74	6.52E-7	1.98E-6	4.94E-6	
UO-31	0.658	1.988	1.756	1.802	0.217	-0.005	-0.035	83	86	-67	-100	-100	1.72E-7	3.65E-7	7.74E-7	
Prostate Cancer																
PC-3	0.525	2.327	2.176	2.251	0.935	0.295	0.377	92	96	23	-44	-28	4.23E-7	2.19E-6	> 1.00E-4	
DU-145	0.888	3.077	3.024	3.114	2.684	0.083	0.383	98	102	82	-91	-57	1.53E-6	2.99E-6	5.82E-6	
Breast Cancer																
MCF7	0.517	2.347	2.179	2.144	0.934	0.185	0.189	91	89	23	-64	-64	3.87E-7	1.83E-6	6.85E-6	
MDA-MB-231/ATCC	0.686	1.726	1.662	1.775	0.929	0.181	0.487	94	105	23	-74	-29	4.71E-7	1.74E-6		
HS 578T	1.444	2.521	2.338	2.451	1.745	0.735	1.172	83	93	28	-49	-19	4.60E-7	2.30E-6	> 1.00E-4	
BT-549	0.928	2.093	2.015	2.090	0.484	0.380	0.734	93	100	-48	-59	-21	2.17E-7	4.74E-7		
T-47D	0.994	2.307	2.153	2.230	1.313	0.563	0.571	88	94	24	-43	-43	4.29E-7	2.28E-6	> 1.00E-4	
MDA-MB-468	0.779	1.485	1.410	1.500	0.641	0.170	0.264	89	102	-18	-78	-66	2.72E-7	7.12E-7	3.42E-6	



