SUPPORTING INFORMATION

Sequoiamonascins A-D : Novel Anticancer Metabolites Isolated from a Redwood Endophyte

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Sequoiamonascin A (1)

*13-120C13
2ac delay*

Figure S2. ^{13}C NMR spectrum of Sequoiamonascin A (1) (in CDCl_3)

Figure S3. ^1H NMR spectrum of Sequoiamonascin B (4) (in CDCl_3)

Figure S4. ^{13}C NMR spectrum of Sequoiamonascin B (4) (in CDCl_3)

Sequoiamonascin C (5)

Figure S5. ¹H NMR spectrum of Sequoiamonascin C (5) (in CDCl₃)

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Figure S7. ^1H NMR spectrum of Sequoiamonascin D (7) (in CDCl_3)

Figure S8. ^{13}C NMR spectrum of Sequoiamonascin D (7) (in CDCl_3)

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Figure S11. NCI human cell line testing data-Mean Graphs for Sequoiamonascin A (1)

National Cancer Institute Developmental Therapeutics Program																
In-Vitro Testing Results																
NSC: D- 722298 / 1				Experiment ID: 0111NS34-10				Test Type: 08				Units: Molar				
Report Date: June 11, 2002				Test Date: November 13, 2001				QNS:				MC:				
COMI:				Stain Reagent: SRB Dual-Pass				SSPL:								
Panel/Cell Line	Time Zero	Ctrl	Mean Optical Densities					Log10 Concentration					Percent Growth	GI50	TGI	LC50
			-8.0	-7.0	-6.0	-5.0	-4.0	-8.0	-7.0	-6.0	-5.0	-4.0				
Leukemia																
CCRF-CEM	0.433	2.166	2.078	2.032	1.647	0.910	0.200	95	92	70	28	-54	2.96E-06	2.18E-05	8.98E-05	
HL-60(TB)	0.194	0.985	1.001	1.001	0.796	0.185	0.151	102	102	76	-5	-22	2.10E-06	8.70E-06	>1.00E-04	
K-562	0.224	1.022	0.965	0.851	0.859	0.427	0.285	93	79	80	25	8	3.52E-06	>1.00E-04	>1.00E-04	
MOLT-4	0.126	0.531	0.541	0.513	0.513	0.209	0.146	103	96	96	21	5	4.05E-06	>1.00E-04	>1.00E-04	
RPMT-8226	0.165	0.529	0.470	0.477	0.456	0.135	0.089	84	86	80	-18	-46	2.02E-06	6.53E-06	>1.00E-04	
SR	0.192	0.706	0.696	0.625	0.527	0.183	0.179	98	84	65	-5	-7	1.65E-06	8.57E-06	>1.00E-04	
Non-Small Cell Lung Cancer																
A549/ATCC	0.227	0.871	0.851	0.844	0.847	0.561	0.048	97	96	96	52	-79	1.03E-05	2.49E-05	6.01E-05	
ERVX	0.591	1.309	1.319	1.327	1.303	1.278	0.062	101	103	99	96	-90	1.76E-05	3.29E-05	6.12E-05	
HOP-92	0.796	1.173	1.129	1.119	1.076	0.914	0.091	88	86	74	31	-89	3.67E-06	1.82E-05	4.77E-05	
NCI-H23	0.378	0.737	0.715	0.670	0.706	0.654	0.035	94	81	91	77	-91	1.45E-05	2.87E-05	5.71E-05	
NCI-H322M	0.700	1.499	1.483	1.474	1.480	1.422	0.203	98	97	98	90	-71	1.78E-05	3.63E-05	7.41E-05	
NCI-H460	0.170	0.982	0.972	0.933	0.908	0.889	0.095	99	94	91	89	-44	1.95E-05	4.63E-05	>1.00E-04	
NCI-H522	0.604	1.027	1.048	0.995	0.999	0.922	-0.019	105	93	93	75	-100	1.39E-05	2.69E-05	5.18E-05	
Colon Cancer																
COLO 205	0.223	1.213	1.254	1.202	1.167	0.807	0.093	104	99	95	59	-59	1.19E-05	3.18E-05	8.46E-05	
HCT-116	0.067	0.495	0.484	0.522	0.500	0.263	0.033	97	106	101	46	-51	8.41E-06	2.98E-05	9.82E-05	
HCT-15	0.281	0.850	0.805	0.792	0.714	0.473	0.049	92	90	76	34	-83	4.13E-06	1.95E-05	5.24E-05	
HT29	0.148	0.798	0.765	0.787	0.735	0.448	0.011	95	98	90	46	-93	8.16E-06	2.15E-05	4.93E-05	
KM12	0.365	1.288	1.279	1.325	1.229	0.830	0.105	99	104	94	50	-71	1.01E-05	2.59E-05	6.67E-05	
SW-620	0.232	1.143	1.103	1.151	1.071	0.478	0.095	96	101	92	27	-59	4.43E-06	2.06E-05	7.85E-05	
CNS Cancer																
SF-268	0.478	1.187	1.146	1.145	1.140	0.979	0.340	94	94	93	71	-29	1.61E-05	5.12E-05	>1.00E-04	
SF-295	0.433	1.288	1.262	1.357	1.331	1.242	0.138	97	108	105	95	-68	1.88E-05	3.81E-05	7.73E-05	
SF-539	0.471	1.229	1.261	1.221	1.206	0.924	0.083	104	99	97	60	-82	1.17E-05	2.63E-05	5.92E-05	
SNB-19	0.282	1.317	1.317	1.360	1.300	1.218	0.144	100	104	98	90	-49	1.95E-05	4.45E-05	>1.00E-04	
U251	0.310	1.139	1.121	1.188	1.083	0.964	0.055	98	106	93	79	-82	1.51E-05	3.09E-05	6.31E-05	
Melanoma																
LOX IMVI	0.287	1.054	1.094	1.015	0.918	0.364	0.036	105	95	82	10	-87	2.79E-06	1.27E-05	4.13E-05	
MALME-3M	0.886	1.552	1.510	1.557	1.551	1.545	0.192	94	101	100	99	-78	1.89E-05	3.62E-05	6.92E-05	
SK-MEL-2	0.518	1.183	1.285	1.335	1.286	0.995	-0.007	115	123	115	72	-100	1.34E-05	2.62E-05	5.11E-05	
SK-MEL-28	0.316	0.863	0.798	0.824	0.773	0.668	-0.003	88	93	83	64	-100	1.22E-05	2.46E-05	4.96E-05	
SK-MEL-5	0.514	1.821	1.756	1.792	1.722	1.392	0.024	95	98	92	67	-95	1.28E-05	2.59E-05	5.26E-05	
UACC-257	0.805	1.793	1.735	1.730	1.611	1.638	0.018	94	94	82	84	-98	1.54E-05	2.90E-05	5.46E-05	
UACC-62	0.832	1.239	1.220	1.193	1.230	0.903	0.157	95	89	98	17	-81	3.92E-06	1.50E-05	4.82E-05	
Ovarian Cancer																
IGROV1	0.312	0.854	0.839	0.796	0.713	0.565	-0.027	97	89	74	47	-100	7.51E-06	2.08E-05	4.56E-05	
OVCA-3	0.491	0.965	0.963	0.935	0.921	0.803	0.135	100	94	91	66	-73	1.30E-05	2.99E-05	6.87E-05	
OVCA-4	0.402	0.916	0.832	0.828	0.798	0.717	0.040	84	83	77	61	-90	1.19E-05	2.54E-05	5.44E-05	
OVCA-5	0.355	0.653	0.619	0.603	0.618	0.594	0.012	88	83	88	80	-97	1.48E-05	2.84E-05	5.45E-05	
OVCA-8	0.295	0.759	0.801	0.750	0.738	0.579	0.106	109	98	95	61	-64	1.23E-05	3.07E-05	7.70E-05	
SK-OV-3	0.401	1.449	1.390	1.445	1.447	1.406	0.394	94	100	100	96	-2	2.95E-05	9.60E-05	>1.00E-04	
Renal Cancer																
A498	1.014	1.531	1.518	1.575	1.523	1.522	0.042	98	108	99	98	-96	1.77E-05	3.21E-05	5.81E-05	
ACHN	0.446	1.230	1.167	1.173	1.129	1.026	-0.006	92	93	87	74	-100	1.37E-05	2.66E-05	5.16E-05	
CAKI-1	0.634	1.368	1.432	1.392	1.398	1.234	0.015	109	103	104	82	-98	1.50E-05	2.85E-05	5.42E-05	
RFP 393	0.545	1.040	1.019	1.057	1.048	0.857	0.073	96	103	102	63	-87	1.22E-05	2.64E-05	5.69E-05	
SN12C	0.618	1.807	1.789	1.716	1.688	1.423	0.054	98	92	90	68	-91	1.29E-05	2.66E-05	5.50E-05	
TK-10	0.844	1.301	1.310	1.316	1.219	1.200	0.050	102	103	82	78	-94	1.45E-05	2.83E-05	5.54E-05	
UO-31	0.344	1.134	1.164	1.156	1.123	1.008	-0.002	104	103	99	84	-100	1.53E-05	2.86E-05	5.35E-05	
Prostate Cancer																
PC-3	0.221	1.126	1.135	1.094	1.018	0.899	0.031	101	96	88	75	-86	1.43E-05	2.92E-05	5.96E-05	
DU-145	0.337	0.723	0.756	0.788	0.729	0.637	-0.019	108	117	101	78	-100	1.43E-05	2.73E-05	5.23E-05	
Breast Cancer																
MCF7	0.265	0.785	0.776	0.812	0.773	0.530	0.106	98	105	98	51	-60	1.02E-05	2.87E-05	8.10E-05	
NCI/ADR-RES	0.392	0.827	0.788	0.803	0.821	0.785	0.123	91	95	99	90	-69	1.79E-05	3.70E-05	7.64E-05	
MDA-MB-231/ATCC	0.697	1.021	0.951	0.931	0.967	0.873	0.059	78	72	83	54	-92	1.07E-05	2.36E-05	5.19E-05	
HS 578T	0.579	1.100	1.085	1.099	1.058	0.937	0.451	97	100	92	69	-22	1.61E-05	5.70E-05	>1.00E-04	
MDA-MB-435	0.409	1.144	1.128	1.125	1.089	0.940	0.224	98	97	93	72	-45	1.55E-05	4.12E-05	>1.00E-04	
MDA-N	0.463	1.694	1.668	1.733	1.637	1.369	0.325	98	103	95	74	-30	1.69E-05	5.15E-05	>1.00E-04	
BT-549	0.605	0.798	0.784	0.743	0.742	0.555	0.062	92	71	71	-8	-90	1.84E-06	7.85E-06	3.24E-05	
T-47D	0.065	1.096	1.050	1.069	1.054	0.874	0.291	96	97	96	78	22	3.19E-05	>1.00E-04	>1.00E-04	

Figure S12. NCI human cell line testing data for Sequoiamonascin A (1)

Figure S13. NCI human cell line testing data-Mean Graphs for Sequoiamonascin B (2)

National Cancer Institute Developmental Therapeutics Program In-Vitro Testing Results																
NSC: D-722299 / 1			Experiment ID: 0111NS34-11			Test Type: 08			Units: Molar							
Report Date: June 11, 2002			Test Date: November 13, 2001			QNS:			MC:							
COMI:			Stain Reagent: SRB Dual-Pass			SSPL:										
Panel/Cell Line	Time Zero	Ctrl	Log10 Concentration					Percent Growth					GI50	TGI	LC50	
			-8.0	-7.0	-6.0	-5.0	-4.0	-8.0	-7.0	-6.0	-5.0	-4.0				
Leukemia																
CCRF-CEM	0.433	2.180	2.083	2.021	2.050	1.852	0.460	94	91	93	81	2	2.46E-05	>1.00E-04	>1.00E-04	
HL-60(TB)	0.194	1.079	1.119	1.102	1.125	1.044	0.188	104	103	105	96	-3	2.91E-05	9.31E-05	>1.00E-04	
K-562	0.224	1.304	1.317	1.296	1.335	1.242	0.206	101	99	103	94	-8	2.71E-05	8.35E-05	>1.00E-04	
MOLT-4	0.126	0.661	0.666	0.619	0.650	0.595	0.237	101	92	98	88	21	3.65E-05	>1.00E-04	>1.00E-04	
RPMT-8226	0.165	0.549	0.534	0.532	0.468	0.406	0.139	96	96	79	63	-32	1.37E-05	4.63E-05	>1.00E-04	
SR	0.192	1.087	0.867	0.838	0.767	0.516	0.203	75	72	64	36	1	3.21E-06	>1.00E-04	>1.00E-04	
Non-Small Cell Lung Cancer																
A549/ATCC	0.227	0.882	0.864	0.885	0.899	0.785	0.339	97	101	103	85	17	3.29E-05	>1.00E-04	>1.00E-04	
EXVX	0.591	1.351	1.324	1.353	1.294	1.214	0.764	96	100	92	82	23	3.47E-05	>1.00E-04	>1.00E-04	
HOP-62	0.187	0.463	0.400	0.422	0.391	0.395	0.238	77	85	74	75	18	2.77E-05	>1.00E-04	>1.00E-04	
HOP-92	0.796	1.179	1.131	1.133	1.060	1.105	0.666	87	88	69	80	-16	2.07E-05	6.78E-05	>1.00E-04	
NCI-H123	0.378	0.712	0.693	0.725	0.723	0.634	0.348	94	104	103	77	-8	2.06E-05	8.06E-05	>1.00E-04	
NCI-H322M	0.700	1.570	1.544	1.566	1.495	1.456	0.752	97	100	91	87	6	2.86E-05	>1.00E-04	>1.00E-04	
NCI-H460	0.170	1.144	1.096	1.097	1.106	0.972	0.351	95	95	96	82	19	3.21E-05	>1.00E-04	>1.00E-04	
NCI-H522	0.604	1.163	1.149	1.175	1.120	1.125	0.401	97	102	92	93	-34	2.19E-05	5.43E-05	>1.00E-04	
Colon Cancer																
COLO 205	0.223	1.158	1.183	1.170	1.238	1.080	0.382	103	101	109	92	17	3.61E-05	>1.00E-04	>1.00E-04	
HCT-116	0.067	0.566	0.512	0.534	0.487	0.471	0.117	89	94	84	81	10	2.73E-05	>1.00E-04	>1.00E-04	
HCT-15	0.281	0.993	0.949	0.991	0.924	0.912	0.327	94	100	90	89	6	2.95E-05	>1.00E-04	>1.00E-04	
HT29	0.148	0.986	1.034	0.987	1.004	0.879	0.354	106	100	102	87	25	3.92E-05	>1.00E-04	>1.00E-04	
KM12	0.365	1.437	1.403	1.449	1.420	1.259	0.345	97	101	98	83	-5	2.37E-05	8.68E-05	>1.00E-04	
SW-620	0.232	1.115	1.125	1.070	1.076	0.981	0.252	101	95	95	85	2	2.64E-05	>1.00E-04	>1.00E-04	
CNS Cancer																
SP-268	0.478	1.219	1.092	1.159	1.153	1.081	0.391	83	92	91	81	-18	2.06E-05	6.55E-05	>1.00E-04	
SP-295	0.433	1.170	1.096	1.150	1.147	1.122	0.516	90	97	97	94	11	3.38E-05	>1.00E-04	>1.00E-04	
SP-539	0.471	1.257	1.216	1.232	1.244	1.170	0.330	95	97	98	89	-30	2.12E-05	5.60E-05	>1.00E-04	
SNB-19	0.282	1.358	1.393	1.314	1.323	1.310	0.625	103	96	97	96	32	5.19E-05	>1.00E-04	>1.00E-04	
SNB-75	0.452	0.680	0.674	0.654	0.647	0.635	0.395	98	89	85	80	-13	2.12E-05	7.30E-05	>1.00E-04	
U251	0.310	1.288	1.273	1.302	1.331	1.225	0.447	98	101	104	94	14	3.53E-05	>1.00E-04	>1.00E-04	
Melanoma																
LOX IMVI	0.287	1.190	1.177	1.296	1.162	1.144	0.176	99	112	97	95	-39	2.16E-05	5.12E-05	>1.00E-04	
MALME-3M	0.886	1.564	1.525	1.590	1.494	1.438	0.842	94	104	90	81	-5	2.31E-05	8.75E-05	>1.00E-04	
M14	0.184	0.484	0.476	0.474	0.461	0.416	0.182	97	97	92	77	-1	2.22E-05	9.61E-05	>1.00E-04	
SK-MEL-2	0.518	1.465	1.430	1.513	1.379	1.288	0.476	96	105	91	81	-8	2.24E-05	8.12E-05	>1.00E-04	
SK-MEL-28	0.316	1.073	1.061	1.042	1.044	1.001	0.393	98	96	96	90	10	3.19E-05	>1.00E-04	>1.00E-04	
SK-MEL-5	0.514	1.686	1.707	1.589	1.543	1.417	0.305	102	92	88	77	-41	1.70E-05	4.51E-05	>1.00E-04	
UACC-257	0.805	1.811	1.894	1.878	1.978	1.817	0.995	108	107	117	101	19	4.16E-05	>1.00E-04	>1.00E-04	
UACC-62	0.832	1.210	1.199	1.252	1.205	1.126	0.377	97	111	99	78	-55	1.62E-05	3.86E-05	9.22E-05	
Ovarian Cancer																
IGROV1	0.312	0.875	0.900	0.921	0.856	0.863	0.306	104	108	97	98	-2	3.01E-05	9.57E-05	>1.00E-04	
OVCAR-3	0.491	0.920	0.927	0.973	0.908	0.871	0.122	102	112	97	89	-75	1.72E-05	3.48E-05	7.02E-05	
OVCAR-4	0.402	1.075	1.035	1.092	1.063	1.002	0.478	94	103	98	89	11	3.18E-05	>1.00E-04	>1.00E-04	
OVCAR-5	0.355	0.628	0.611	0.621	0.611	0.595	0.273	94	97	94	88	-23	2.19E-05	6.19E-05	>1.00E-04	
OVCAR-8	0.295	0.799	0.796	0.756	0.858	0.741	0.106	100	92	112	89	-64	1.79E-05	3.80E-05	8.07E-05	
SK-OV-3	0.401	1.375	1.346	1.331	1.367	1.345	0.863	97	96	99	97	47	8.86E-05	>1.00E-04	>1.00E-04	
Renal Cancer																
786-O	0.151	0.431	0.385	0.395	0.379	0.362	0.198	84	87	82	75	17	2.71E-05	>1.00E-04	>1.00E-04	
A498	1.014	1.585	1.633	1.665	1.604	1.562	0.947	109	114	103	96	7	2.81E-05	8.61E-05	>1.00E-04	
ACHN	0.446	1.375	1.291	1.417	1.428	1.337	0.800	91	104	106	96	38	6.21E-05	>1.00E-04	>1.00E-04	
CAKI-1	0.634	1.376	1.301	1.371	1.294	1.338	0.315	90	99	89	95	-50	2.04E-05	4.50E-05	9.95E-05	
RXFT 393	0.545	1.082	1.047	1.059	0.997	1.001	0.408	94	96	84	85	-25	2.07E-05	5.90E-05	>1.00E-04	
SN12C	0.618	1.812	1.673	1.711	1.628	1.543	0.432	88	92	85	77	-30	1.80E-05	5.25E-05	>1.00E-04	
TK-10	0.844	1.462	1.414	1.443	1.404	1.401	0.885	92	97	91	90	7	3.02E-05	>1.00E-04	>1.00E-04	
UO-31	0.344	1.411	1.338	1.302	1.284	1.301	0.519	93	90	88	90	16	3.48E-05	>1.00E-04	>1.00E-04	
Prostate Cancer																
PC-3	0.221	1.147	1.103	1.124	1.115	1.068	0.507	95	98	97	91	31	4.83E-05	>1.00E-04	>1.00E-04	
DU-145	0.337	0.751	0.720	0.756	0.763	0.742	0.353	92	101	103	98	4	3.22E-05	>1.00E-04	>1.00E-04	
Breast Cancer																
MCF7	0.265	0.907	0.918	0.931	0.867	0.841	0.309	102	104	94	90	7	3.01E-05	>1.00E-04	>1.00E-04	
NCI/ADR-RES	0.392	0.826	0.838	0.832	0.809	0.792	0.401	103	101	96	92	2	2.94E-05	>1.00E-04	>1.00E-04	
MDA-MB-231/ATCC	0.697	1.021	0.978	0.948	0.900	0.953	0.407	87	77	63	79	-42	1.74E-05	4.52E-05	>1.00E-04	
HS 578T	0.579	1.112	1.118	1.125	1.105	1.008	0.629	101	102	99	81	9	2.68E-05	>1.00E-04	>1.00E-04	
MDA-MB-435	0.409	1.179	1.149	1.206	1.148	1.113	0.282	96	104	96	91	-31	2.18E-05	5.58E-05	>1.00E-04	
MDA-N	0.463	1.726	1.739	1.681	1.675	1.570	0.487	101	96	96	88	2	2.75E-05	>1.00E-04	>1.00E-04	
BT-549	0.605	0.819	0.770	0.808	0.933	0.747	0.269	77	95	153	66	-56	1.36E-05	3.50E-05	9.01E-05	
T-47D	0.065	1.123	1.079	1.067	1.015	1.055	0.456	96	95	90	94	37	5.87E-05	>1.00E-04	>1.00E-04	

Figure S14. NCI human cell line testing data for Sequoiamonascin B (2)