Supplemental Materials

Cytotoxic triterpenes from *Salacia crassifolia* and metabolite profiling of Celastraceae species

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CDCl_{3.}

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(S1) Cytotoxicity of *S. crassifolia* root wood hexane extract in colon COLO205 and KM12; renal A498 and U031; osteosarcoma MG63 and MG63.3 cancer cell lines.

Developmental Thera	peutics Program	NSC: D-N192803/	Test Date: Mar 16, 2015	
One Dose Bar	Graph	Experiment ID: 150	3OS49	Report Date: Jul 01, 2015
Panel/Cell Line	Growth Percent	Bar Graph		
Leukemia				
HL-60(TB)	-52.15			
SR	-27.28			—
Non-Small Cell Lung Cancer				
A549/ATCC	-63.86			
HOP-62	-79.95			
HOP-92	-89.81			
NCI-H226 NCI-H23	-26.46			
NCI-H322M	-69.77			
NCI-H460	-54.96			
Colon Cancer	-00.00			
HCC-2998	-80.46			
HCT-116	-73.21			
HC1-15 HT29	-72.98			
KM12	-73.56			
SW-620	-46.25			
SF-268	-63 45			
SF-539	-77.61			
SNB-19	-45.63			
U251	-70.72			
Melanoma				
LOX IMVI	-72.14			
MALME-SM M14	-51.75			
MDA-MB-435	-66.00			
SK-MEL-2 SK-MEL-28	-/3./9 -45.37			
SK-MEL-5	-66.39			
UACC-62	-76.39			
OVCAR-3	-83.21			
OVCAR-4	-69.22			
OVCAR-5	-61.93			
NCI/ADR-RES	-61.94			
SK-OV-3	-94.15			
Renal Cancer 786-0	-67 47			
A498	-80.35			
ACHN	-74.26			
BXF 393	-63.57 -51.57			
SN12C	-33.64			-
TK-10	-84.64			
Prostate Cancer	-11.55			
PC-3	-83.42			
DU-145 Breast Cancer	-83.72			
MCF7	-68.31			
HS 578T	-30.17			
B1-549 T-47D	-82.02			
MDA-MB-468	-39.23			-
	-			
	1	00 50	0.0	-50 -100
			rercentage Growth	1

(S2) NCI-60 single dose bar graph of *S. crassifolia* root wood extract.

Developmental Therapeutics Program			NSC: D-N192803 / 1 Conc: 1.00E2 ug/ml		Test	Test Date: Mar 16, 2015	
One Dose Mean Graph			Experiment ID: 1503OS49 Report Date: Jul 01, 2015			ul 01, 2015	
Panel/Cell Line	Growth Percent	Me	an Growth	Percent - Growth F	ercent		
Leukemia HL-60(TB)	-52.15			_			
MOLT-4 SR	-38.11 -27.28						
Non-Small Cell Lung Cancer A549/ATCC	-63.86						
EKVX HOP-62	-85.85 -79.95						
HOP-92	-89.81						
NCI-H220 NCI-H23	-20.40 -70.52		· •	-			
NCI-H322M	-69.77						
NCI-H460 NCI-H522	-54.96						
Colon Cancer	-00.00			[
HCC-2998	-80.46						
HCT-116 HCT-15	-72.98						
HT29	-62.99			•			
KM12	-73.56						
CNS Cancer	-40.20						
SF-268	-63.45						
SNB-19	-77.61						
SNB-75	-76.78						
U251	-70.72			-			
LOX IMVI	-72.14			-			
MALME-3M	-63.74			_			
M14 MDA-MB-435	-51./5						
SK-MEL-2	-73.79			-			
SK-MEL-28	-45.37						
UACC-62	-76.39			-			
Ovarian Cancer	02.01						
OVCAR-3 OVCAR-4	-69.22			- F			
OVCAR-5	-61.93						
OVCAR-8 NCI/ADB-BES	-74.14 -61.94			- E -			
SK-OV-3	-94.15						
Renal Cancer 796.0	.87.47						
A498	-80.35						
ACHN	-74.26						
RXF 393	-83.57 -51.57						
SN12C	-33.64						
TK-10	-84.64						
Prostate Cancer	-11.55						
PC-3	-83.42						
Breast Cancer	-63.72						
MCF7	-68.31						
HS 5781 BT-549	-30.17 -82.02						
T-47D	-34.20						
MDA-MB-468	-39.23						
Mean	-65.44						
Delta	28.71		.				
Lange	07.08						
						100	
	150	100	50	0	-50	-100	-150

(S3) NCI-60 single dose mean bar graph of *S. crassifolia* root wood extract.



(S4) NCI-60 dose response curves for S. crassifolia root wood extract.

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National Cancer Institute Developmental Therapeutics Program			NSC :N192803/1	Units :ug/ml	SS	SPL :	EXP. ID :1506FS98
Mean Graphs F			Report Date :July 01, 2015	Report Date :July 01, 2015			l.
Panel/Cell Line	Log ₁₀ GI50 G	150	Log ₁₀ TGI T	GI	Log ₁₀ L(C50 LC50	1
Leukemia CCRF-CEM HL-80(TB) K-562 MOLT-4 RPMI-8226 SR SR	-0.56 -0.71 -0.59 -0.76 -0.775	Ē	-0.14 -0.18 -0.06 -0.29 -0.14 -0.23		^ 1.222	.00 .84 .00 .00 .00 .00	
A 540/ACCC EKVX HOP-92 HOP-92 NGLH228 NGLH228 NGLH228 NGLH228 NGLH228 NGLH322M NGLH322M NGLH322M	0.15 -0.29 -0.34 -0.46 -0.48 -0.49 -0.49 -0.49 -0.32 -0.32 -0.73		0.50 0.22 0.21 -0.06 0.64 0.64 0.43 0.25 -0.26		0 0 0 0 0 0 0 0 0	.84 .63 .55 .62 .73 .74 .44	
Colon Cancer COLC 205 HCC-2998 HCT-116 HCT-16 HCT-16 KM12 SW-620 CNS Cancer	0.54 0.497 0.778 0.78 0.54 -0.23 -0.53	F	0.08 0.05 -0.46 -0.48 0.09 0.32 -0.03		0 0. -0. -0. 0. 0.	181 16 16 17 188 177 62	=
SF-268 SF-295 SF-539 SNB-19 SNB-75 U251 Welanoma	-0.51 -0.17 -0.26 -0.27 -0.23 -0.58	}	0.10 0.31 0.24 0.27 0.29 -0.23		0. 0. 0. 0. 0. 0.	.67 .69 .65 .71 .76 .34	
LOX IMVI MALME-3M MDA-MB-435 SK-MEL-2 SK-MEL-28 SK-MEL-28 UACC-257 UACC-257 UACC-257 UACC-257 UACC-257	-0.77 -0.59 -0.65 -0.53 -0.42 -0.47 -0.30 -0.43 -0.48		-0.50 -0.15 -0.26 0.03 0.22 0.22 0.22 0.23 0.15 0.03		-u. 0. 0. 0. 0. 0. 0.	222 57 29 55 55 60 60 62 93 58	
OVCAR-3 OVCAR-3 OVCAR-4 OVCAR-5 OVCAR-5 NCI/ADR-RES SK-OV-3 Renal Cancer	-0.61 -0.75 -0.48 -0.08 -0.50 -0.50 -0.55 -0.15		-0.20 -0.45 -0.15 -0.41 -0.07 -0.03 -0.45	-	0. -0. 0. 0. 0. 0.	.49 116 164 174 169 1.74	-
788-0 A498 ACHN CAKI-1 RXF 393 RXF 393 TK-0 UC-31 Proteita Cancer	-0.71 0.04 -0.74 -0.44 -0.62 -0.77 -0.77 -0.77 -0.73		-0.42 0.37 -0.44 0.09 -0.38 0.05 -0.18 -0.30		-0. -0. -0. -0. 0. 0.	.13 .70 .14 .57 .14 .63 .44	
PC-3 DU-145	-0.46 -0.50		0.11 0.06		0.	.69 .57	
MCF-MB-231/ATCC MCA-MB-231/ATCC HT-549 T-470 MDA-MB-468	-0.55 -0.69 -0.31 -0.316 -0.75 -0.71	Ę	0.05 -0.31 0.28 0.13 -0.27 -0.36	-	> 2 > 2	.59 .26 .00 .61 .00	-
_MID Delta Range	-0.47 0.31 1.14	<u> </u>	0.0 0.5 1.14	<u> </u>	0.7 0.92 2.22		
	+3 +2 +1	0 -1 -2 -3	+3 +2 +1 () -1 -2 -3		+3 +2 +1 0	-1 -2 -3

(S5) NCI-60 5-dose mean bar graph of *S. crassifolia* root wood extract.





(S6) NCI-60 cumulative dose response curves for *S. crassifolia* root wood extract.





(S7) Cytotoxicity of DIOL fractions A-E of *S. crassifolia* root wood hexane extract in renal A498 and U031 cancer cell lines.





S. crassifolia Diol Fraction E





(S8) Cytotoxicity of DIOL fractions A-E of *S. crassifolia* root wood hexane extract in osteosarcoma MG63 and MG63.3 cell lines.







(S9) Cytotoxicity of DIOL fractions A-E of *S. elliptica* root wood ethyl acetate extract in renal A498 and U031 cancer cell lines.







(S10) Cytotoxicity of DIOL fractions A-E of *S. elliptica* root wood ethyl acetate extract in osteosarcoma MG63 and MG63.3 cell lines.





(S11) HRESIMS spectrum of 11β -hydroxypristimerin (1).



(S12) Infrared spectrum of 11β -hydroxypristimerin (1).



(S13) UV spectrum of 11β -hydroxypristimerin (1).



(S14) ¹H NMR spectrum (600 MHz) of 11β-hydroxypristimerin (**1**) in CDCl₃.



(S15) 13 C NMR spectrum (150 MHz) of 11 β -hydroxypristimerin (1) in CDCl₃.





(S16) COSY spectrum of 11β -hydroxypristimerin (1) in CDCl₃.



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(S17) HSQC spectrum of 11β -hydroxypristimerin (1) in CDCl₃.

(S18) HMBC spectrum of 11β -hydroxypristimerin (1) in CDCl₃.

	11β-Hydroxypristimerin						
	(Compound 1)						
	С	Н					
С							
2	178.8	-					
3	145.9	-					
4	118.0	-					
5	128.6	-					
8	167.2	-					
9	48.1	-					
10	161.6	-					
13	40.6	-					
14	44.9	-					
17	30.87	-					
20	40.4	-					
29	178.7	-					
CH							

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1	121.6	7.32 (s)
6	132.2	6.88 (d, 7.2)
7	118.8	6.28 (d, 7.2)
11	65.3	4.57 (dd, 12.2, 6.4)
18	43.9	1.59 (m)
CH ₂		
12	43.4	2.38 (m); 2.01 (m)
15	28.7	1.62 (m); 1.58 (m)
16	36.2	1.87 (m); 1.51 (m)
19	30.81	2.40 (m); 1.74 (m)
21	29.7	2.24 (m); 1.40 (m)
22	34.3	2.00 (m); 0.98 (m)
23	10.4	2.19 (s)
CH ₃		
25	34.4	1.64 (s)
26	21.4	1.30 (s)
27	18.5	0.61 (s)
28	31.4	1.10 (s)
30	32.7	1.20 (s)
MeO	51.8	3.60 (s)

(S19) NMR Spectroscopic Data (¹H 600 MHz, ¹³C 150 MHz) for 11β -hydroxypristimerin (**1**) in CDCl₃.

(S20) Chromatogram, MS1 and MS2 spectra of the LC-MS/MS analysis of pristimerin (**2**).

(S21) ¹H NMR spectrum (600 MHz) of pristimerin (2) in CDCl₃.

(S22) ¹³C NMR spectrum (150 MHz) of pristimerin (2) in CDCl₃.

(S23) COSY spectrum of pristimerin (2) in CDCl₃.

(S24) HSQC spectrum of pristimerin (2) in CDCl₃.

Pristimerin ([1], [2], [3])

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4.1) 5.0, 2.0) 1.71 (m) 1.68 (m) 1.68 (td, 13.0, 4.5) 1.68 (td, 13.0, 4.5) 15 28.65 1.67 (td, 13.9, 28.7) 1.66 (td, 14.0, 5.5) 28.7 28.68 1.70 (m) 28.4 15 28.65 1.67 (td, 14.4, 36.4) 1.56 (td, 14.0, 6.0, 2.0) 1.60 (m) 1.60 (m) 28.4 16 36.39 1.89 (td, 14.4, 36.4) 1.88 (td, 14.0, 6.0) 36.4 36.25 1.88 (m) 36.3 1.51 (dd, 14.4, 5.5, 2.0) 1.51 (dd, 14.4, 5.5, 2.0) 5.5, 2.0) 1.51 (dd, 14.4, 5.5, 2.0) 1.53 (m) 1.53 (m)
1.68 (m) 1.68 (td, 13.0, 4.5) 28.6 1.70 (m) 28.4 15 28.65 1.67 (td, 13.9, 28.7) 1.66 (td, 14.0, 5.5) 28.7 28.68 1.70 (m) 28.4 16 36.39 1.89 (td, 14.4, 36.4) 1.88 (td, 14.0, 6.0) 36.4 36.25 1.88 (m) 36.3 1.51 (dd, 14.4, 5.5, 2.0) 1.51 (dd, 14.4, 5.5, 2.0) 1.53 (m) 1.53 (m) 1.53 (m)
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16 36.39 1.89 (td, 14.4, 36.4 1.86 (td, 14.0, 6.0) 36.4 36.25 1.88 (tf) 36.3 6.1) 1.50 (ddd, 14.0, 1.50) 1.50 (ddd, 14.0, 1.50) 1.51 (dd, 14.4, 1.55, 2.0) 1.53 (tf) 1.53 (tf)
1.51 (dd, 14.4, 5.5, 2.0)
1.31 (dd, 14.4, 5.3, 2.0)
19 30.91 2.43 (br.d. 15.0 30.9 30.94 2.24 (dl 30.9
$\begin{array}{c ccccccccccccccccccccccccccccccccccc$
1 71 (dd 15.9) 1 69 (dd 15.0)
8.2) 8.0)
21 29.89 2.21 (m) 29.9 2.20 (ddd, 14.0, 29.9 29.86 2.21 (dl. 29.8
1.39 (td, 14.4, 4.5, 2.0)
4.6) 1.38 (td, 14.0, 4.0) 1.38 (dt)
22 34.81 2.06 (td, 14.4, 34.8 2.05 (td, 14.0, 4.5) 34.8 34.77 2.04 (m) 34.8
3.6) 0.98 (ddd, 14.0, 0.99 (dl.
0.98 (br d) 4.0, 2.0) 13.9)
CH ₃

23	10.23	2.22 (s)	10.2	2.21 (s)	10.2	2.21 (s)	10.70	2.29 (s)	13.6
25	38.29	1.46 (s)	38.3	1.45 (s)	38.3	1.45 (s)	38.29	1.48 (s)	37.6
26	21.60	1.27 (s)	21.6	1.26 (s)	21.4	1.26 (s)	21.07	1.29 (s)	20.6
27	18.35	0.54 (s)	18.3	0.53 (s)	18.3	0.53 (s)	18.53	0.52 (s)	18.3
28	31.61	1.11 (s)	31.6	1.10 (s)	31.6	1.10 (s)	31.60	1.11 (s)	31.5
30	32.69	1.19 (s)	32.7	1.18 (s)	32.7	1.18 (s)	32.59	1.18 (s)	32.9
MeO	51.57	3.56 (s)	51.6	3.55 (s)			51.67	3.56 (s)	51.1

(S25) NMR Spectroscopic Data (¹H 600 MHz, ¹³C 150 MHz) for pristimerin (**2**) in CDCl₃.

(S26) Chromatogram, MS1 and MS2 spectra of the LC-MS/MS analysis of 6oxopristimerol (**3**).

(S27) ¹H NMR spectrum (600 MHz) of 6-oxopristimerol (3) in CDCl₃.

(S28) ¹³C NMR spectrum (150 MHz) of 6-oxopristimerol (3) in CDCl₃.

(S29) COSY spectrum of 6-oxopristimerol (3) in CDCl₃.

(S30) HSQC spectrum of 6-oxopristimerol (3) in CDCl₃.

164B107H 4 1 F:\164B107H

167B107H_HSQC_CDC13

(S31) HMBC spectrum of 6-oxopristimerol (3) in CDCl₃.

6-Oxopristimerol J. Nat. Prod. **1994**, 57(12), 1675 **3-O-methyl-6-oxopristimerol** *Chemistry & biodiversity* **2011**, *8*, 2291

	HS	HSQC HMBC 6-Oxopristimerol, em C ₅ D ₅ N		НМВС		3-O-methyl-6-Oxopristimerol , CDCl ₃		
	С	Н	² Jch	³ J _{CH}	С	Н	С	Н
C								
2	147.99	-	H-1		144.04	-	144.2	-
3	141.00	-		H-1; 3H-23	126.80	-	132.9	-
4	125.30	-	3H- 23		122.67	-	132.0	-
5	122.33	-		H-1; H-7; 3H-23	151.38	-	154.9	-
6	188.44	-			187.32	-	187.2	-
8	172.99	-		3H-25; 3H- 26	150.67	-	151.9	-
9	40.55	-	3H- 25		40.58	-	40.4	-
10	151.51	-	H-1	3H-25	170.77	-	171.2	-
13	39.12	-	3H- 27	3H-26	39.30	-	38.9	-
14	44.75	-	3H- 26	3H-27	44.61	-	44.7	-
17	30.96	-	3H- 28		30.64	-	30.8	-
20	40.55	-	3H- 30		40.14	-	40.3	-
29	179.52	-		3H-30; MeO- 29	178.66	-	178.8	-
СН								
1	108.89	6.98 (s)			109.99	7.25 (s)	109.1	6.95 (s)
6	-	-	-	-	-	-	-	-
7	125.12	6.46 (s)			126.88	6.46 (s)	126.1	6.14 (s)
18	44.27	1.60		3H-27; 3H- 28	44.38	1.58	44.3	
CH ₂								
11	34.00	2.14, 1.83		3H-25	34.59		34.0	2.21, 1.94
12	29.73	1.84, 1.27		3H-27	30.21		29.8	1.72, 1.66
15	28.50	1.70, 1.59		3H-26	28.86		28.5	1.80, 1.40
16	36.34	1.88, 1.52		3H-28	36.62		36.4	1.80, 1.50
19	30.51	2.14, 1.69		3H-30	31.08		30.5	2.91 (d, 15.9), 1.66

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21	29.89	2.20,		3H-30	30.11		29.7	2.19, 1.37
		1.40						
22	34.82	2.04,		3H-28	35.13		34.8	2.04, 0.97
		0.98						
CH ₃								
23	13.68	2.67 (s)			14.82	3.28 (s)	14.7	2.66 (s)
25	37.63	1.46 (s)			37.76	1.53 (s)	37.6	1.55 (s)
26	20.69	1.27 (s)			20.87	1.16 (s)	20.8	1.29 (s)
27	18.31	0.53 (s)			18.51	0.63 (s)	18.3	0.57 (s)
28	31.58	1.10 (s)			31.55	0.99 (s)	31.6	1.09 (s)
30	32.87	1.18 (s)			32.59	1.15 (s)	32.7	1.17 (s)
MeO-	51.70	3.55 (s)			51.47	3.58 (s)	51.5	3.57 (s)
29								
MeO-3	-	-	-	_	-	-	61.1	3.79 (s)

(S32) NMR Spectroscopic Data (^{1}H 600 MHz, ^{13}C 150 MHz) for 6-oxopristimerol

(3) in CDCl₃.

(S33) MS2 Mass spec of vitideasin (4).

(S34) ¹H NMR spectrum (600 MHz) of vitideasin (4) in CDCl₃.

(S35) ¹³C NMR spectrum (150 MHz) of vitideasin (4) in CDCl₃.

(S36) COSY spectrum of vitideasin (4) in CDCl₃.

(S37) HSQC spectrum of vitideasin (4) in CDCl₃.

(S38) HMBC spectrum of vitideasin (4) in CDCl₃.

	Vitideas	in (Compound 4)		
	С	Н		
С				
2	178.0	-		
3	146.2	-		
4	116.7	-		
5	127.5	-		
8	159.7	-		
9	44.5	-		
10	160.13	-		
13	43.1	-		
14	135.3	-		
15	128.3	-		
17	33.7	-		
20	42.6	-		
29	179.3	-		
СН				
1	119.9	6.59 (s)		
6	134.9	7.19 (d, 7.0 Hz)		
7	121.6	6.17 (d, 7.0 Hz)		
11	37.5	1.93 - 2.00 (m)		
18	43.9	1.40 - 1.48 (m)		
CH ₂				
12	35.6	2.54 (ddd);		
		1.3 (overlapped)		
16	37.8	2.65 (d); 1.28		
		(overlapped)		
19	33.9	1.54 (t); 1.68-1.71 (m)		
21	28.6	1.46 - 1.48 (m);		
		1.85 - 1.93 (m)		
22	36.1	1.64 (m)		
CH ₃				
23	10.3	2.2 (s)		
25	29.4	1.3 (m)		
26	21.9	1.73 (s)		
27	24.0	0.82 (s)		
28	31.5	1.20 (s)		
30	19.8	1.21 (s)		
MeO	51.8	3.68 (s)		
OH		7.09 (bs)		

(S39) NMR Spectroscopic Data (¹H 600 MHz, ¹³C 150 MHz) for vitideasin (4) in CDCl₃.

	S. crassifolia NSC:N192803 Endpt:GI50 Expld:AVGDATA hiConc:2.0	S. elliptica NSC:N192805 Endpt:GI50 Expld:AVGDATA hiConc:2.0
S. crassifolia NSC:N192803 Endpt:GI50 Expld:AVGDATA hiConc:2.0	1.0	0.749
S. elliptica NSC:N192805 Endpt:GI50 Expld:AVGDATA hiConc:2.0	0.749	1.0
	S. crassifolia NSC:N192803 Endpt:TGI Expld:AVGDATA hiConc:2.0	S. elliptica NSC:N192805 Endpt:TGI Expld:AVGDATA hiConc:2.0
S. crassifolia NSC:N192803 Endpt:TGI Expld:AVGDATA hiConc:2.0	1.0	0.807
S. elliptica NSC:N192805 Endpt:TGI Expld:AVGDATA hiConc:2.0	0.807	1.0
	S. crassifolia NSC:N192803 Endpt:LC50 Expld:AVGDATA hiConc:2.0	S. elliptica NSC:N192805 Endpt:LC50 Expld:AVGDATA hiConc:2.0
S. crassifolia NSC:N192803 Endpt:LC50 Expld:AVGDATA hiConc:2.0	1.0	0.765
<i>S. elliptica</i> NSC:N192805 Endpt:LC50 Expld:AVGDATA hiConc:2.0	0.765	1.0

(S40) COMPARE between *S. crassifolia* and *S. elliptica* extracts.

	PRISTIMERIN NSC:S791208 Endpt:GI50 Expld:AVGDATA hiConc:-4.0	11B-HYDROXY- PRISTAMERIN NSC:S797253 Endpt:GI50 Expld:AVGDATA hiConc:-4.1	S. elliptica NSC:N192805 Endpt:GI50 Expld:AVGDA TA hiConc:2.0
PRISTIMERIN NSC:S791208 Endpt:GI50 Expld:AVGDATA hiConc:-4.0	1.0	0.518	0.692
11B-HYDROXY- PRISTAMERIN NSC:S797253 Endpt:GI50 Expld:AVGDATA hiConc:-4.1	0.518	1.0	0.642
S. elliptica NSC:N192805 Endpt:GI50 Expld:AVGDATA hiConc:2.0	0.692	0.642	1.0
	PRISTIMERIN NSC:S791208 Endpt:TGI Expld:AVGDATA hiConc:-4.0	11B-HYDROXY- PRISTAMERIN NSC:S797253 Endpt:TGI Expld:AVGDATA hiConc:-4.1	S. elliptica NSC:N192805 Endpt:TGI Expld:AVGDA TA hiConc:2.0
PRISTIMERIN NSC:S791208 Endpt:TGI Expld:AVGDATA NConc:-4.0	1.0	0.557	0.813
11B-HYDROXY- PRISTAMERIN NSC:S797253 Endpt:TGI Expld:AVGDATA hiConc:-4.1	0.557	1.0	0.578
S. elliptica NSC:N192805 Endpt:TGI Expld:AVGDATA hiConc:2.0	0.813	0.578	1.0
	PRISTIMERIN NSC:S791208 Endpt:TGI Expld:AVGDATA hiConc:-4.0	11B-HYDROXY- PRISTAMERIN NSC:S797253 Endpt:TGI Expld:AVGDATA hiConc:-4.1	S. elliptica NSC:N192805 Endpt:TGI Expld:AVGDA TA hiConc:2.0
PRISTIMERIN NSC:8791208 Endpt:LC50 Expld:AVGDATA hiConc:-4.0	1.0	0.745	0.86
11B-HYDROXY- PRISTAMERIN NSC:S797253 Endpt:LC50 Expld:AVGDATA hiConc:-4.1	0.745	1.0	0.749
S. elliptica NSC:N192805 Endpt:LC50 Expld:AVGDATA hiConc:2.0	0.86	0.749	1.0

(S41) COMPARE between *S. elliptica* extracts, pristimerin (2) and 11β -hydroxypristimerin (1).

Developmental Therapeutics Program		NSC: D-N192805 / 1 Conc: 1.00E2 ug/ml		Test Date: Mar 16, 2015	
One Dose Bar Graph		Experiment ID: 1503OS49 Report Date: Jul 0			
Panel/Cell Line	Growth Percent	Bar Graph			
Leukemia					
HL-60(TB)	-48.99				
MOLT-4	-37.09			<u> </u>	
SR	-37.17			-	
Non-Small Cell Lung Cancer	76.22				
A049/ATCC	-/6.33				
HOP-62	-88.04				
HOP-92	-85.71				
NCI-H226	-43.46				
NCI-H23	-73.13				
NCI-H322M	-76.78				
NCI-H460	-00.27				
Colon Cancer	-00.95				
HCC-2998	-83 23				
HCT-116	-72 72				
HCT-15	-85.95				
HT29	-80.47				
KM12	-71.25				
SW-620	-60.82				
SE-268	-70.86				
SF-539	-76.42				
SNB-19	-67.32				
SNB-75	-45.35			<u> </u>	
U251	-80.36				
Melanoma					
LOX IMVI	-89.23				
MALME-3M M14	-03.40				
MDA-MB-435	-77 45				
SK-MEL-2	-70.01				
SK-MEL-28	-62.80				
SK-MEL-5	-81.82				
UACC-62	-80.87				
OVCAR-3	-90.42				
OVCAR-4	-75.03				
OVCAR-5	-76.79				
OVCAR-8	-73.94				
NCI/ADR-RES	-79.37				
SK-OV-3 Banal Canaar	-93.58				
786-0	-77 24				
A498	-92.12				
ACHN	-88.83				
CAKI-1	-87.39				
RXF 393	-65.07				
SNI2C	-07.60				
UO-31	-89.49				
Prostate Cancer					
PC-3	-80.41				
DU-145	-91.77				
Breast Cancer	05.42				
MCF/ HS 578T	-00.43				
BT-549	-64.50				
T-47D	-65.78				
MDA-MB-468	-58.02				
	1	100 50	0.0	-50 -100	
			Percentage Growt	a	

(S42) NCI-60 single dose bar graph of *S. elliptica* root wood extract.

Developmental Therapeutics Program		NSC: D-N192805 / 1 Conc: 1.00E2 ug/ml	Test Date: Mar 16, 2015	
One Dose Mean Graph		Experiment ID: 1503OS49	Report Date: Jul 01, 2015	
Panel/Cell Line	Growth Percent	Mean Growth Percent - Growth Per	rcent	
Panev/Cen Line Leukemia HL-80(TB) MOLT-4 SR Non-Small Cell Lung Cancer A549/ATCC EKVX HOP-82 HOP-92 NCI-H226 NCI-H228 NCI-H228 NCI-H322 Colon Cancer HCC-2998 HCT-116 HCT-115 HT29 KM12 SW-620 CNS Cancer SF-268 SF-539 SNB-19 SNB-75 U251 Melanoma LOX IMVI MALME-3M M14 MDA-MB-435 SK-MEL-2 SK-MEL-2 SK-MEL-2 SK-MEL-2 SK-MEL-2 SK-MEL-2 SK-MEL-2 SK-MEL-2 SK-MEL-2 SK-MEL-2 SK-MEL-5 UACC-62 Ovarian Cancer OVCAR-3 OVCAR-4 OVCAR-4 OVCAR-5 OVCAR-5 OVCAR-8 NCI/ADR-RES SK-OV-3 Renal Cancer 788-0 A498 ACHN CAKI-1 RXF 393 SN12C TK-10 UO-31 Prostate Cancer PC-3 DU-145 Breast Cancer MCF7 HS 578T BT-549 T-47D MDA-MB-468	Growth Percent -48.99 -37.09 -37.17 -76.33 -94.08 -88.04 -85.71 -43.46 -73.13 -76.78 -55.27 -80.95 -83.23 -72.72 -85.95 -80.47 -71.25 -60.82 -70.86 -70.86 -80.42 -67.32 -45.35 -80.36 -89.23 -65.46 -56.74 -77.45 -70.01 -62.80 -81.82 -80.87 -90.42 -75.03 -75.03 -77.74 -70.73 -93.58 -77.24 -92.12 -88.83 -87.39 -65.76 -92.63 -89.49 -80.41 -91.77 -85.43 -36.32 -65.76 -80.32 -65.76 -92.63 -89.49 -80.41 -91.77 -85.43 -36.32 -65.76 -80.32 -65.76 -80.41 -91.77 -85.43 -36.32 -65.76 -80.32 -65.76 -80.41 -91.77 -85.43 -36.32 -65.76 -80.32 -65.76 -80.32 -65.76 -80.41 -91.77 -85.43 -36.32 -65.76 -80.32 -65.76 -80.32 -65.76 -80.41 -91.77 -85.43 -36.32 -65.76 -80.32 -65.76 -80.32 -65.76 -80.32 -65.76 -80.41 -91.77 -85.43 -36.32 -65.76 -80.32 -65.76 -80.32 -65.76 -80.32 -65.76 -80.32 -65.76 -80.32 -65.76 -80.32 -65.76 -80.32 -65.76 -80.32 -65.76 -80.32 -65.76 -80.32 -65.76 -80.41 -91.77 -85.43 -36.32 -65.76 -80.32 -65.76 -80.32 -80.57 -77.24 -91.77 -85.43 -36.32 -65.76 -80.32 -77.24 -91.77 -85.43 -36.32 -65.76 -80.32 -77.24 -91.77 -85.43 -36.32 -65.76 -80.32 -77.24 -91.77 -85.43 -36.32 -85.02 -77.24 -72.04			
Mean Delta Range	-73.04 21.04 57.76			
	150	100 50 0 -50	0 -100 -150	

(S43) NCI-60 single dose mean bar graph of *S. elliptica* root wood extract.

(S44) NCI-60 dose response curves for *S. elliptica* root wood extract.

National Cancer Institute Developmental Therapeutics Program		NSC :N192805/1	NSC :N192805/1 Units :ug/ml		EXP. ID :1506FS98	
	Mean Graphs		Report Date :July 01, 2015		Test Date :June 08, 2015	
Panel/Cell Line	Log ₁₀ GI50	GI50	Log ₁₀ TGI TG	âl	Log ₁₀ LC50 LC5	D
Leukemia CCRF-CEM HL-80(TB) K-562 MOLT-4 RPMI-8226 NOS Bandl Cell Lung Cappor	0.30 0.35 0.40 -0.13 0.34 0.34	l_	0.75 0.78 0.80 0.55 0.78 0.61	:	> 2.00 1.88 > 2.00 > 2.00 > 2.00 > 2.00 > 2.00	
Advance Advance Edva HOP-82 HOP-82 NCI-H23 NCI-H23 NCI-H460 NCI-H460 NCI-H522 Colon Cancer	0.50 0.9 0.31 0.70 0.29 0.64 0.28 0.31		1.00 0.82 0.68 1.29 0.66 1.20 0.66 1.20 0.60 0.58		1.64 1.50 0.96 1.96 1.96 1.92 1.63 0.92 0.86	
COLC 205 HCC-2998 HCT-116 HCT-115 HCT-15 HCT-15 HCT-15 HCT-15 CM12 SW-620 CNS Cancer	0.28 0.23 0.14 0.15 0.41 0.41 0.31		0.85 0.55 0.46 0.45 0.75 1.01 0.70		1.31 0.87 0.75 1.28 1.63 1.34	=
SF-288 SF-295 SF-539 SNB-19 SNB-75 U251 Melanoma	0.32 0.23 0.39 0.40 0.57 0.21		0,79 0,64 0,72 0,84 1,09 0,52	-	1.51 1.12 1.18 1.50 1.76 0.82	-
LDX INVI M1AME-3M M1AME-3M M1A-MB-435 SK-MEL-2 SK-MEL-2 SK-MEL-2 SK-MEL-5 UACC-25 UACC-25 UACC-25 UACC-25 UACC-25	0.17 0.36 0.17 0.29 0.50 0.39 0.27 0.44 0.25		0.46 0.66 0.53 0.66 0.82 0.74 0.56 0.77 0.62		0.74 0.96 0.88 1.10 1.53 1.34 0.85 1.38 0.99	5
OVGAR-3 OVCAR-3 OVCAR-4 OVCAR-5 OVCAR-5 OVCAR-5 NC/ADR-RES SK-OV-3 Renal Cancer	0.32 0.18 0.22 0.49 0.37 0.33 0.54		0.64 0.46 0.71 0.92 0.75 0.75 1.00	-	0.97 0.75 1.42 1.55 1.44 1.65 1.54	-
786-0 A498 ACHN CAKI-1 FIXF 393 SN12C TK-10 UC-31 C-21	0.23 0.46 0.17 0.30 0.27 0.42 0.42 0.22 0.02		0.51 0.84 0.47 0.72 0.52 0.89 0.59 0.59 0.37		0.78 1.38 0.76 1.29 0.78 1.59 0.96 0.72	
PC-3 DU-145	0.44 0.25	1	0.94 0.60		1.62 0.94	
Heast Cancer MCF7 MDA-MB-231/ATCC HS 578T BT-549 T-47D MDA-MB-468	0.33 0.22 0.52 0.37 -0.11 0.19	{	0.75 0.67 1.11 0.70 0.45 0.52	-	1.44 > 2.00 1.12 0.94 0.85	
_MID Delta Range	0.31 0.44 0.83 +3 +2 +1	0 -1 -2 -3	0.71 0.34 0.92 +3 +2 +1 0		1.29 0.57 1.28 +3 +2 +1 0	-1 -2 -3

(S45) NCI-60 5-dose mean bar graph of *S. elliptica* root wood extract.

(S46) NCI-60 cumulative dose response curves for *S. elliptica* root wood extract.

(S47) NCI-60 dose response curves for 11β -hydroxypristimerin (1).

National Cancer Institute Dev	velopmental Therapeutics	Program	NSC : D - 797253/1	Units Molar	SSPL:0GZS	EXP. ID :1705NS01
Mean Graphs		Report Date :June 16, 2017		Test Date :May 08, 2017		
Panel/Cell Line	Log_GI50	GI50	Log, TGI TGI		Log_LC50 LC50	
Leukemia CCRF-CEM HL-60(TB) K-562 MOLT-4 RPMI-6226 SR Non Sall Cell Lung Cancer AS49/ATCC CEVX	-5.56 -5.01 -5.37 -5.50 -5.59 -5.57 -4.89	E	4.93 4.54 4.54 4.70 4.56 4.70 4.72 4.72	-	4.10 4.10 4.10 4.10 4.10 4.10 4.10 4.10 4.10 4.10	
HOP-62 HOP-92 NCH-1226 NCH-1232M NCH-1322M NCH-1460 NCH-1522 Colon, Canger	-4.88 -4.94 -4.86 -4.87 -4.87 -4.87 -5.08		4.59 4.63 4.65 4.55 4.50 4.59 4.70		-4.30 -4.33 -4.35 -4.23 -4.32 -4.32 -4.32 -4.32 -4.32	
COLC 2998 HCI-116 HCI-15 HT29 KM12 SW-620 CNS Cancer	-2.13 -4.89 -5.44 -5.29 -4.97 -4.89 -5.03		4.60 4.84 4.75 4.64 4.69		-4.13 -4.42 -4.33 -4.33 -4.33 -4.32 -4.36	
SF-268 SF-295 SF-539 SNB-19 SNB-75 U251 Melanoma	-5.02 -4.88 -4.80 -4.91 -4.93 -5.06		465 455 454 452 459 477	1	-4.29 -4.21 -4.38 -4.34 -4.24 -4.40	
MALME-3M MIA MDA-MB-435 SK-MEL-28 SK-MEL-28 SK-MEL-29 UACC-62 Ovarian Cancer			4.579 4.657 4.667 4.67 4.67 4.67 4.61 4.61 4.51 4.72		4.37 4.30 4.36 4.32 4.39 4.19 4.23 4.38	
IGROVI OVCAR-3 OVCAR-4 OVCAR-5 OVCAR-5 NCI/ADR-RES SK-OV-3 Renal Cancer	-5.17 -5.06 -5.08 -4.89 -4.83 -4.82 -4.72		4.72 4.73 4.71 4.61 4.55 4.46 4.37		-4.31 -4.40 -4.33 -4.33 -4.26 -4.10 > -4.10	
785-0 ACHN CAKI-1 RXF 393 SN12C TK-10 UO-31 Prograde Cancer	-5.75 -5.42 -5.40 -4.95 -5.02 -5.32 -5.32 -5.24		-5.28 -4.87 -4.86 -4.64 -4.68 -4.68 -4.79		-4.66 -4.48 -4.48 -4.34 -4.34 -4.34 -4.43 -4.43	
PC-3 DU-145 Breast Cancer	-5.06 -4.91		-4.72 -4.63		-4.38 -4.36	
MCF7 MDA-MB-231/ATCC HS 578T BT-549 T-47D MDA-MB-468	-4.95 -4.99 -4.82 -4.98 -5.52 -5.01	-	-4.62 -4.66 -4.42 -4.65 -4.80 -4.66		-4.30 -4.33 > 4.10 -4.24 -4.24 -4.31	
MID	-5.06		-4.55 0.52		43	

(S48) NCI-60 5-dose mean bar graph of 11β -hydroxypristimerin (1).

(S49) NCI-60 cumulative dose response curves for 11β -hydroxypristimerin (1).

(S50) NCI-60 dose response curves for pristimerin (2).

National Cancer Institute Developmental Therapeutics Program		NSC : D - 791208/1	Units :Molar	SSPL :0W3X	EXP. ID :1607NS41
	Mean Graphs	Report Date :September 13	3, 2016	Test Date July 11, 2016	
Panel/Cell Line	Log ₁₀ GI50 GI50	Log ₁₀ TGI TG	ai L	.og ₁₀ LC50 LC50)
Leukemia CCRF-CEM HL-80(TB) K-062 MOLT-4 RPMI-8226 SR	-6.68 -6.79 -6.60 -6.79 -6.74 -6.72	-8.13 -8.17 -6.16 -6.28 -6.29 -6.29	-	 → 4.00 → 4.33 → 4.00 → 4.44 → 4.00 	
Non-Small Cell Lung Cancer Ad49/ATCC EKVX HOP-92 HOP-92 NCI-H23 NCI-H23 NCI-H322M NCI-H460 NCI-H622 Colon Cancer	-022 -033 -032 -032 -070 -023 -023 -025 -070	0.00 -0.00 -0.81 -0.41 -0.41 -0.41 -0.72 -0.72 -0.12 -0.30		5.27 5.26 5.36 4.09 5.50 5.36 5.48 5.87	-
COLO 200 HCC-2998 HCT-116 HCT-16 HCT-16 KM12 SW-620	-8.74 -8.68 -8.79 -8.77 -9.68 -9.43 -8.78	-6.36 -6.32 -6.50 -6.38 -6.38 -0.83 -0.83 -6.38		-0.89 -0.89 -0.82 -0.82 -0.82 -0.26 -0.91	
SI-288 SI-295 SI-295 SI-295 SI-295 SI-295 SI-75 U231 Melanoma	- 6.47 - 6.30 - 6.56 - 6.56 - 6.76 - 6.78	-5.91 -5.79 -6.26 -6.03 -6.07 -8.49	-	-0.37 -0.36 -0.81 -0.48 -0.04 -0.04 -0.23	
LOX IMVI MALME-3M MTDA-MD-435 SK-MEL-2 SK-MEL-2 SK-MEL-28 SK-MEL-6 UACC-257 UACC-62 CA	- 6.76 - 6.64 - 6.77 - 6.62 - 6.61 - 6.70 - 6.55 - 6.69	-6.49 -6.33 -6.30 -8.26 -8.22 -6.22 -6.24 -6.12 -6.33		-6.27 -6.07 -6.78 -5.74 -5.71 -5.71 -5.75 -5.65 -5.65 -5.65 -5.50 -5.91	-
OVCAR-3 OVCAR-3 OVCAR-4 OVCAR-6 OVCAR-6 OVCAR-8 NCIADR-RES SK-OV-3 Renal Cancer	-8.70 -8.77 -8.82 -8.36 -8.63 -8.59 -8.11	-8.34 -8.49 -8.47 -6.82 -8.22 -8.18 -6.70		-5.80 -6.83 -6.39 -5.34	-
786-0 A498 ACHN RXF 393 SN12C TK-10 UC-31 Prostate Cancer	-6.76 -0.48 -6.81 -6.75 -6.75 -6.73 -6.73 -6.90	-6.50 -6.03 -6.54 -6.48 -6.48 -6.29 -6.35 -6.58		-6.24 -6.48 -6.26 -6.21 -6.21 -5.75 -5.90 -6.27	
PC-3 DU-145	-6.62 -6.74	-6.24 -6.42	•	-5.69 -6.10	-
Breact Juncer MDC-MB-231/ATCC HDC-MB-231/ATCC HDC-MB-240 T-47D MDA-MB-468	40,99 477 40,244 40,244 40,244 40,900 40,78		,	-6.04 -4.00 -5.52 -6.11	-
_MiD Delta Runge	-6.63 0.27 0.89	-0.22 0.38 0.90	_	554 2.73 2.27	_
	+3 +2 +1 0 -1 -2	-3 +3 +2 +1 0	-1 -2 -3	+3 +2 +1 0	-1 -2 -3

(S51) NCI-60 5-dose mean bar graph of pristimerin (2).

Developmental Therapeutics Program		NSC: D-791209 / 1 Conc: 1.00E-5 Molar		Test Date: Jun 06, 2016	
One Dose Bar Graph		Experiment ID: 1606OS22 Report Date:		Report Date: Jun 26, 2016	
Panel/Cell Line	Growth Percent	Bar Graph			
Leukemia	22.22				
CCRF-CEM HL-60(TB)	26.89				
K-562	48.95				
MOLT-4	18.34				
RPMI-8226	27.04		-		
SR Non-Small Call Lung Concer	51.18				
A549/ATCC	38.57		_		
EKVX	71.68				
HOP-62	71.73				
HOP-92	49.21				
NCLH23	48.04				
NCI-H322M	70.60				
NCI-H460	31.83				
NCI-H522	38.49		•		
COLO 205	71.53				
HCC-2998	76.69				
HCT-116	31.33				
HCT-15	36.85				
H129 KM12	90.17				
SW-620	60.33				
CNS Cancer					
SF-268	61.73				
SF-280 SE-530	49.85				
SNB-19	60.55				
SNB-75	112.13				
0251	41.97				
I OX IMVI	50 73				
MALME-3M	105.72				
M14	66.40				
MDA-MB-430 SK-MEL-2	08.04 71.63				
SK-MEL-28	91.28				
SK-MEL-5	7.93				
UACC-257	41.85				
Ovarian Cancer	20.32		_		
IGROV1	50.77				
OVCAR-3	47.89				
OVCAR-4	47.40				
OVCAR-8	60.43				
NCI/ADR-RES	63.39				
SK-OV-3	58.35				
786-0	78 56				
A498	57.10				
ACHN	53.30				
RXF 393	85.03				
TK-10	68.86				
UO-31	50.56				
Prostate Cancer					
PG-3 DIL145	33.83		-		
Breast Cancer	07.12				
MCF7	41.95		•		
MDA-MB-231/ATCC	61.35				
HS 5/81 BT-540	/9.4/ 82.13				
T-47D	54.10				
MDA-MB-468	30.12				
	1	125 62.5	0.0 Percentage Crowth	-62.5 -125	
			Fercentage Growth		

(S52) NCI-60 cumulative dose response curves for pristimerin (2).

(S53) NCI-60 single dose bar graph of 6-oxopristimerol (3).

Developmental Thera	Developmental Therapeutics Program		NSC: D-791209 / 1 Conc: 1.00E-5 Molar		Test Date: Jun 06, 2016
One Dose Mea	in Graph	Ð	Experiment ID: 1606OS22		Report Date: Jun 26, 2016
Panel/Cell Line	Growth Percent		Mean Growth	Percent - Growth Per	cent
Leukemia CCRF-CEM	26.89				
HL-60(TB)	38.42				
MOLT-4	18.34				
RPMI-8226 SR	27.04 51.18				
Non-Small Cell Lung Cancer	38.57				
EKVX	71.68				
HOP-62 HOP-92	71.73 49.21				
NCI-H226	51.12				
NCI-H322M	70.60				
NCI-H460 NCI-H522	31.83 38.49				
Colon Cancer	71.53				
HCC-2998	76.69				
HCT-116 HCT-15	31.33 36.85				
HT29	90.17				
SW-620	60.33				
CNS Cancer SF-268	61,73				
SF-295	49.85				
SNB-19	60.55				
SNB-75 U251	112.13 41.97		1 T		
Melanoma	50.73				
MALME-3M	105.72		-		
M14 MDA-MB-435	66.40 58.54				
SK-MEL-2	71.63				
SK-MEL-5	7.93				
UACC-257 UACC-62	41.85 28.32				
Ovarian Cancer	50.77				
OVCAR-3	47.89				
OVCAH-4 OVCAR-5	118.52		│ —		
OVCAR-8 NCI/ADR-RES	60.43			1	
SK-OV-3	58.35				
786-0	78.56			—	
A498 ACHN	57.10 53.30				
RXF 393	85.03				
TK-10	68.86				
UO-31 Prostate Cancer	50.56				
PC-3	33.83				
Breast Cancer	07.12				
MCF7 MDA-MB-231/ATCC	41.95 61.35				
HS 578T BT-549	79.47				
T-47D	54.10				
MDA-MB-468	30.12				
Mean	57.23 49.30				
Range	110.59				
	L				
	150	•	100 50	0 -50	-100 -150

(S54) NCI-60 singe dose mean bar graphs of 6-oxopristimerol (3).