#### **Supporting Information**

Synthesis and evaluation of novel anti-cancer compounds derived from the natural product Brevilin A

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Figure S1. Effects of BA compounds on viability of different cancer cells.







Figure S1. Effects of BA compounds on viability of different cancer cells. A549, SW480, MDA-MB-231 and MCF-7 cells were treated with different doses of BA and its analogs for 48 hours. Cell viability was measured by MTT assay. MTT results of (A) A549, (B) SW480, (C) MDA-MB-231, and (D) MCF-7 cells. Data is shown as means  $\pm$  SD; \**P* < 0.05, \*\**P* < 0.01, \*\*\**P* < 0.001 compared to control.

## Purity quality control of BA-1-12

### BA-1,5,12:

HPLC system	Shimazu LC-20AT, coupled with SPD-20A Detector				
Column	Alltima C18, 4.6 x 250 mm, 5 µm or equivalent				
Detector	DAD				
Detector wavelength	223 nm				
Flow rate	1.0 mL/min				
Gradient of mobile phase	Time (min)	% (A) Acetonitrile	% (B) water		
	0	40	60		
	10 80 20				

20

**BA-1:** 



100

0

1 PDA Multi 1 / 223nm 4nm

		Peal	cTable	
PDA Ch1 2	23 nm 4 nm			
Peak#	Ret. Time	Area	Height	Area %
1	13.931	640982	104829	95.501
2	14.196	15326	2576	2.283
3	16.972	5154	837	0.768
4	18.188	9713	1506	1.447
Total		671175	109749	100.000





PeakTable

DA Ch1 22	3nm 4nm			
Peak#	Ret. Time	Area	Height	Area %
1	2.814	1115	231	0.112
2	9.584	987519	138147	99.613
3	12.775	416	76	0.042
4	16.657	1454	90	0.147
5	18.372	851	65	0.086
Total		991355	138608	100.000

**BA-12:** 



1 PDA Multi 1 / 223nm 4nm

]	PDA Ch1 2	23nm 4nm			
	Peak#	Ret. Time	Area	Height	Area %
	1	9.761	199927	24561	98.663
ſ	2	10.585	1929	295	0.952
ſ	3	12.737	780	141	0.385
	Total		202636	24997	100.000

### **BA-2:**

HPLC system	Shimazu LC-20AT, coupled with SPD-20A Detector					
Column	Alltima C18, 4.6 x 250 mm, 5 µm or equivalent					
Detector	DAD					
Detector wavelength	223 nm					
Flow rate	1.0 mL/min					
Gradient of mobile phase	Time (min)% (A) Acetonitrile% (B) water					
	0 38 62					

Time (min)	% (A) Acetonitrile	% (B) water
0	38	62
12	44	56
20	45	55



1						
1						
-						
4						
-						
4						
22						
-						
						9
-						19
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		50	7.6	10.0	12.5	15.0
0.0	2.5	5.0	1.5	10.0	12.5	15.0
Multi 1 / 2	23nm 4nm					

		Peal	Table	
PDA Ch1 2	223nm 4nm			
Peak#	Ret. Time	Area	Height	Area %
1	14.616	2156	181	0.344
2	15.708	624376	42213	99.656
Total		626532	42395	100.000

## BA-3,4,6,9:

HPLC system	Shimazu LC-20AT, coupled with SPD-20A Detector				
Column	Alltima C18, 4.6 x 250 mm, 5 µm or equivalent				
Detector	DAD				
Detector wavelength	223 nm				
Flow rate	1.0 mL/min				
Gradient of mobile phase	Time (min)	% (A) Acetonitrile	% (B) water		
	0	60	40		
	10 90 10				
	20	100	0		

**BA-3:** 



1 PDA Multi 1 / 223nm 4nm

PDA Ch1 22	23nm 4nm			
Peak#	Ret. Time	Area	Height	Area %
1	5.461	982	74	0.125
2	7.680	441	55	0.056
3	10.389	1849	246	0.236
4	11.038	765667	101193	97.786
5	11.232	14067	2475	1.796
Total		783005	104043	100.000

-				
Dool	10	0		0
rea	ΚI	a	U.	le.





PeakTable	

PDA Ch1 22	23nm 4nm			
Peak#	Ret. Time	Area	Height	Area %
1	3.610	2250	149	0.229
2	5.470	2837	162	0.289
3	7.654	1078	114	0.110
4	11.014	971482	133156	99.022
5	17.235	3427	174	0.349
Total		981074	133754	100.000

#### **BA-6:**



D 1				
Pea	κI	a	b.	le

]	PDA Ch1 223nm 4nm					
	Peak#	Ret. Time	Area	Height	Area %	
	1	7.943	1469105	159926	97.925	
	2	15.341	31130	988	2.075	
	Total		1500235	160914	100.000	



PeakTable PDA Ch1 223nm 4nm Ret. Time Peak# Area % Height Area 5.506 4292 0.780 274 1 0.780 98.379 0.232 0.609 23 10.981 541091 76159 17.242 18.402 1274 195 3348 550005 516 77145 4 Total 100.000

## BA-7,8,10,11:

HPLC system	Shimazu LC-20AT, coupled with SPD-20A Detector				
Column	Alltima C18, 4.6 x 250 mm, 5 µm or equivalent				
Detector	DAD				
Detector wavelength	223 nm				
Flow rate	1.0 mL/min				
Gradient of mobile phase	Time (min)	% (A) Acetonitrile	% (B) water		
	0	38	62		
	12	44	56		
	25	47	53		
	30	50	50		
	35	100	0		

40

BA-7:



100

0

1 PDA Multi 1 / 223nm 4nm

PDA Ch1 2	23nm 4nm			
Peak#	Ret. Time	Area	Height	Area %
1	20.681	35428	1891	0.976
2	22.048	7312	409	0.201
3	25.127	76184	3709	2.098
4	27.262	3511495	163360	96.724
Total		3630419	169369	100.000

PeakTable





1 PDA Multi 1 / 223nm 4nm

PeakTable

DA Ch1 22	23nm 4nm			
Peak#	Ret. Time	Area	Height	Area %
1	12.951	4236	306	0.546
2	13.845	11730	627	1.513
3	15.532	2335	170	0.301
4	15.986	3175	219	0.410
5	17.097	746298	47919	96.251
6	19.137	2743	163	0.354
7	27.235	4846	234	0.625
Total		775362	49638	100.000

# **BA-10:**



PDA Ch1 22	23nm 4nm			
Peak#	Ret. Time	Area	Height	Area %
1	27.150	20223	812	1.630
2	29.402	3128	172	0.252
3	37.717	2963	425	0.239
4	38.130	1201200	205702	96.795
5	38.469	1033	154	0.083
6	38.851	6614	793	0.533
7	39.357	5811	1166	0.468
Total		1240971	209223	100.000

Dool	ьт	-1	1	0
Pea.	ΚI	a	)]	e



1 PDA Multi 1 / 223nm 4nm

PDA Ch1 2	23 nm 4 nm			
Peak#	Ret. Time	Area	Height	Area %
1	23.014	10236	562	0.276
2	24.600	2694	150	0.073
3	27.176	23818	1084	0.642
4	27.748	14606	701	0.393
5	29.357	3656522	147965	98.487
6	31.763	2897	132	0.078
7	32.732	1930	139	0.052
Total		3712703	150732	100.000

Peak	[ab	le

#### NMR spectra of BA-1–12

<sup>1</sup>H and <sup>13</sup>C NMR spectra of BA-1 (in CDCl<sub>3</sub>)



<sup>1</sup>H and <sup>13</sup>C NMR spectra of BA-2 (in CDCl<sub>3</sub>)





<sup>1</sup>H and <sup>13</sup>C NMR spectra of BA-4 (in pyridine-*d*<sub>5</sub>)



#### <sup>1</sup>H and <sup>13</sup>C NMR spectra of BA-5 (in CDCl<sub>3</sub>)





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<sup>1</sup>H and <sup>13</sup>C NMR spectra of BA-7 (in CDCl<sub>3</sub>)



<sup>1</sup>H and <sup>13</sup>C NMR spectra of BA-8 (in CDCl<sub>3</sub>)



<sup>1</sup>H and <sup>13</sup>C NMR spectra of BA-9 (in CDCl<sub>3</sub>)



<sup>1</sup>H and <sup>13</sup>C NMR spectra of BA-10 (in CDCl<sub>3</sub>)





<sup>1</sup>H and <sup>13</sup>C NMR spectra of BA-12 (in CDCl<sub>3</sub>)

