Supplementary Data

This supplementary data is a part of a paper entitled "Volatile Organic Compounds and Antioxidant, Cytotoxic Activities of Extracts from the Leaves of *Grewia bulot*".

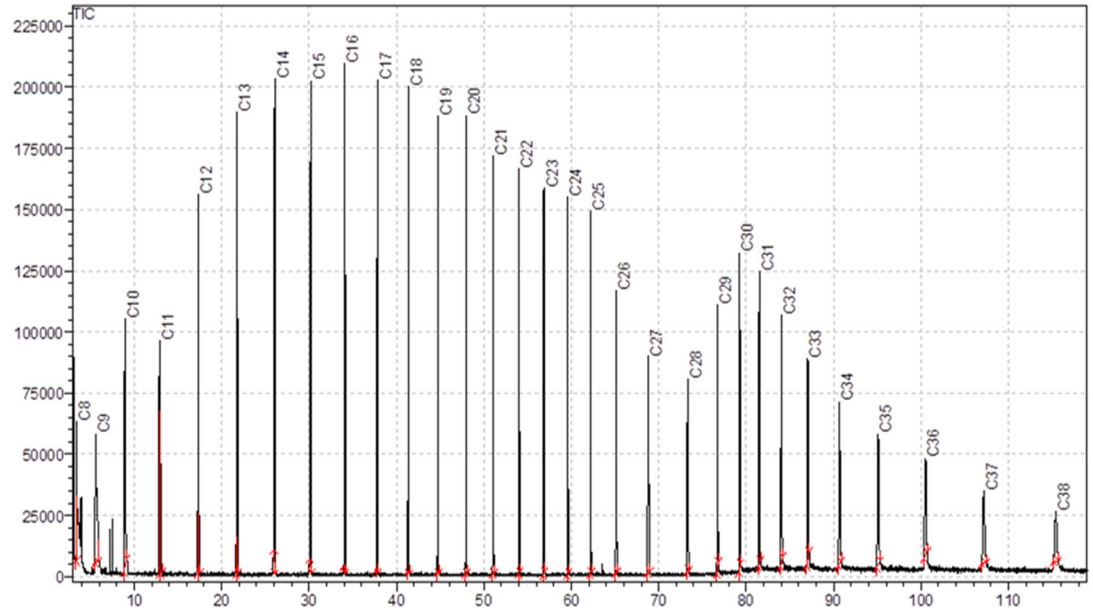

Fig S1. GC-MS data of *n*-alkanes

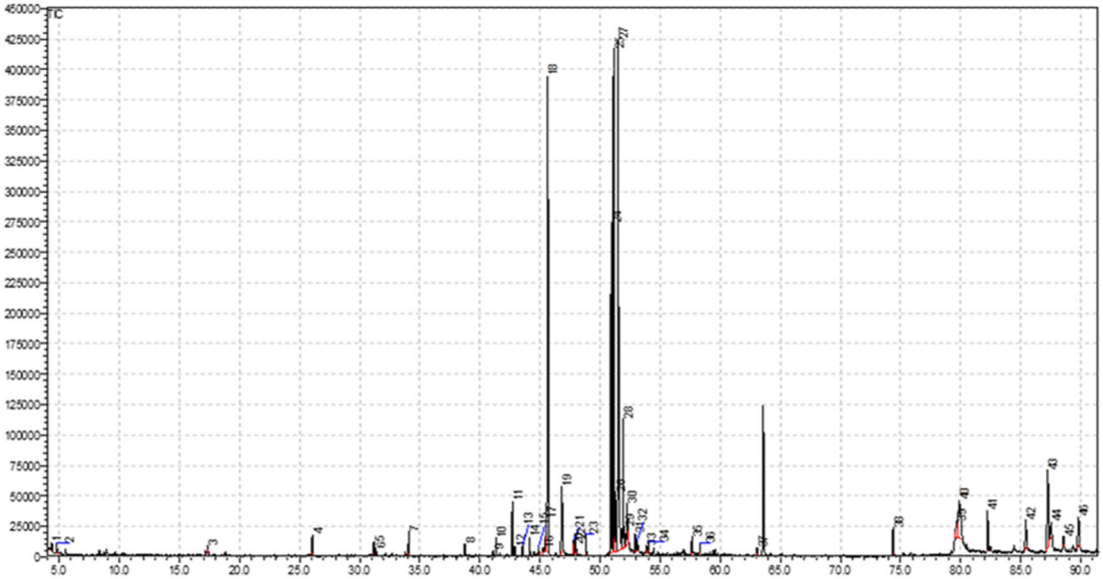

Fig S2. GC-MS data of *n*-hexane fraction

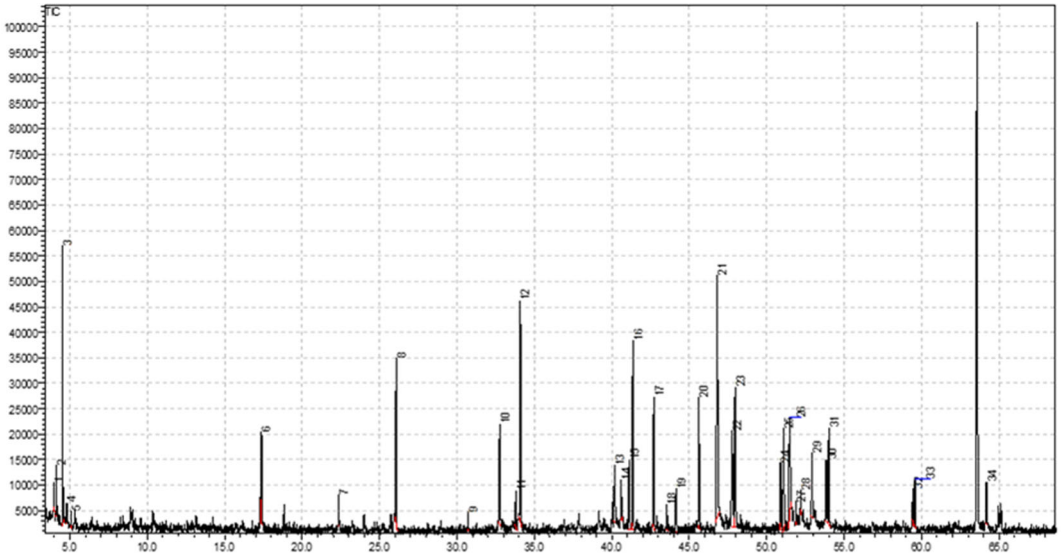

Fig S3. GC-MS data of dichloromethane fraction

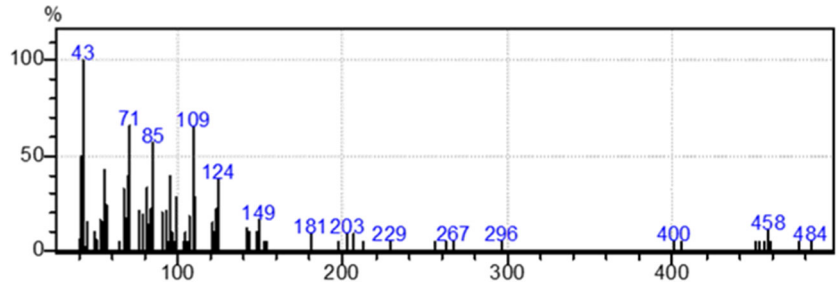

Fig S4. EI-MS of compound 13

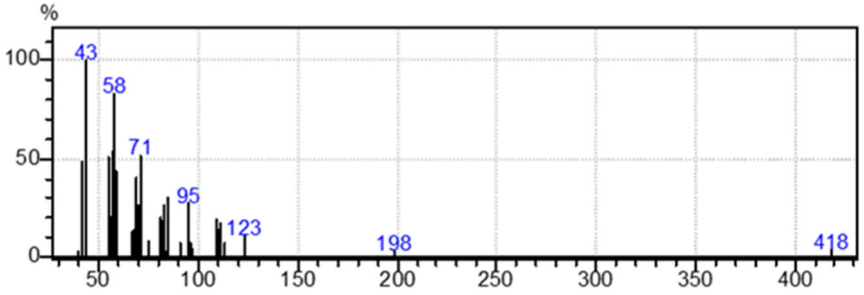

Fig S5. EI-MS of compound 17

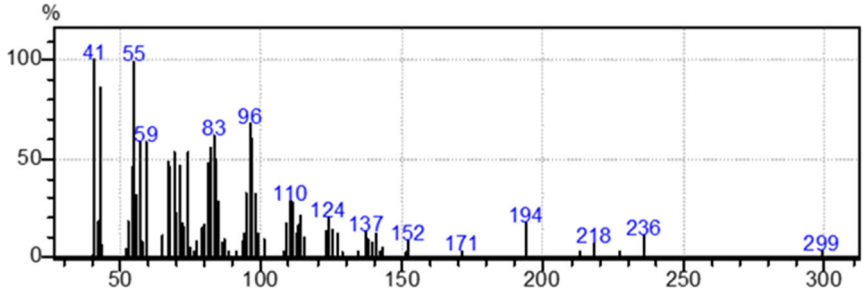

Fig S6. EI-MS of compound 18

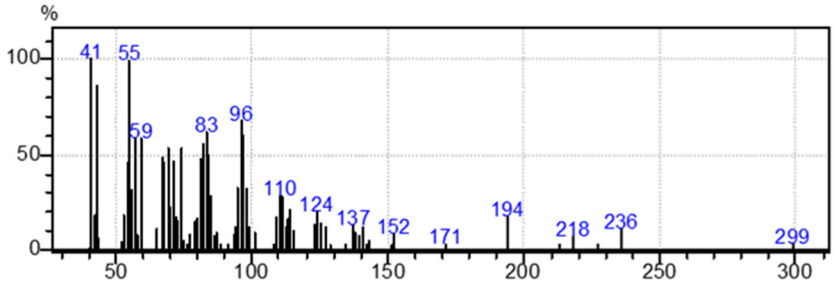

Fig S7. EI-MS of compound 21

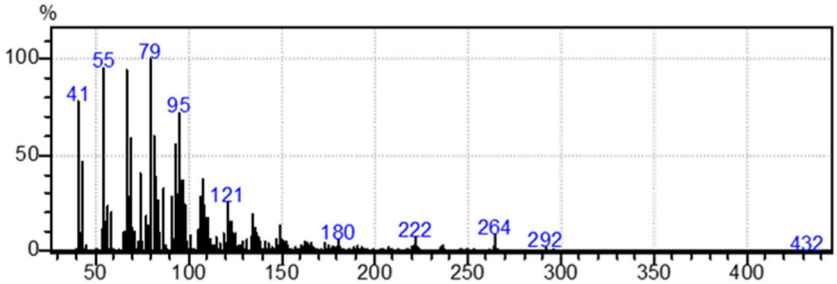

Fig S8. EI-MS of compound 29

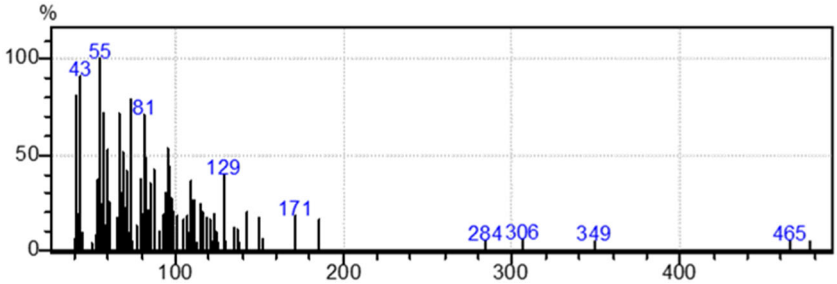

Fig S9. EI-MS of compound 35

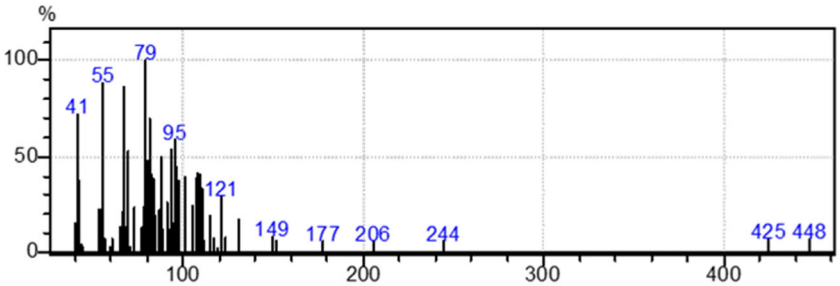

Fig S10. EI-MS of compound 36

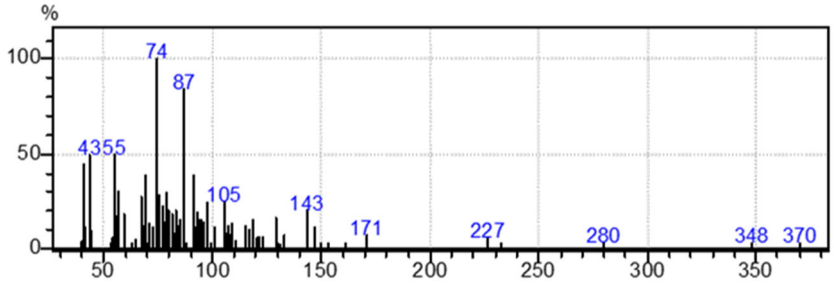

Fig S11. EI-MS of compound 39

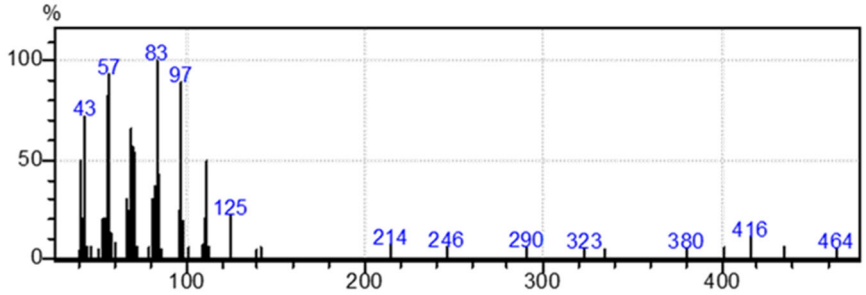

Fig S12. EI-MS of compound 40

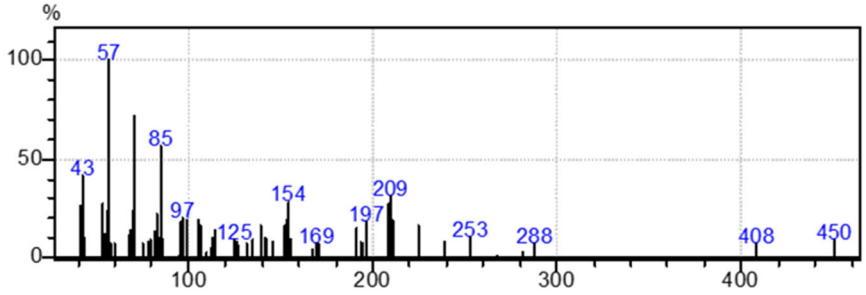

Fig S13. EI-MS of compound 45

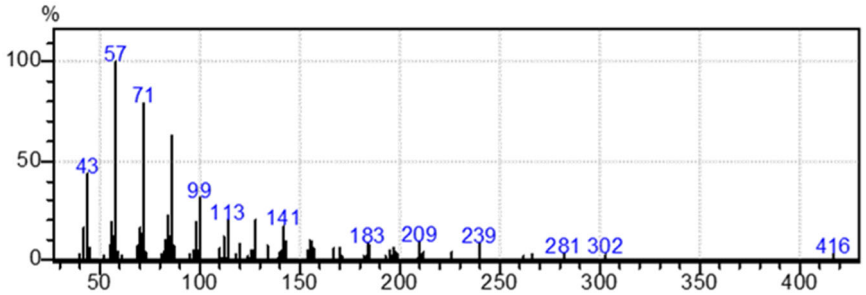

Fig S14. EI-MS of compound 46

Table S1. Volatile compositions (%) of the *n*-hexane and dichloromethane fractions of *Grewia bulot* leaves

No.	RT	Compound[a]	*n*-hexane fraction	Dichloromethane fraction	Identification[b,c]
1	3.95	Isovaleric acid	-	0.9	MS, RI, O
2	4.78	2-*tert*-Butoxyethanol	0.2	5.3	MS, RI, O
3	17.37	Dodecane	0.5	3.4	MS, RI, O
4	22.37	2-Methoxy-4-vinylphenol	-	1.1	MS, RI, O
5	26.06	Tetradecane	0.7	4.9	MS, RI, O
6	31.18	Methyl laurate	0.4	-	MS, RI, O
7	31.35	Dihydroactinidiolide	0.2	-	MS, RI, O
8	32.75	Lauric acid	-	4.0	MS, RI, O
9	33.78	1-Hexadecene	-	1.3	MS, RI, O
10	34.08	Hexadecane	0.8	7.4	MS, RI, O
11	38.75	Methyl tetradecanoate	0.4	-	MS, RI, O
12	40.17	Loliolide	-	2.7	MS, RI, O
13	40.58	Unidentified	-	2.1	MS, RI, O
14	41.11	1-Octadecene	0.1	2.2	MS, RI, O

No.	RT	Compound[a]	*n*-hexane fraction	Dichloromethane fraction	Identification[b,c]
15	41.35	Octadecane	0.5	6.0	MS, RI, O
16	42.71	Phytol	1.4	4.4	MS, RI, O
17	42.92	Unidentified	0.3	-	MS, RI, O
18	43.54	Unidentified	0.3	0.8	MS, RI, O
19	44.14	3,7,11,15-Tetramethyl-2-hexadecen-1-ol	0.5	1.6	MS, RI, O
20	44.91	Methyl oleate	0.2	0.2	MS, RI, O
21	45.49	Unidentified	1.1	-	MS, RI, O
22	45.65	Methyl palmitate	14.4	3.9	MS, RI, O
23	46.83	Palmitic acid	2.9	9.8	MS, RI, O
24	47.77	1-Eicosene	0.6	4.7	MS, RI, O
25	47.82	Ethyl palmitate	0.6	-	MS, RI, O
26	47.97	Eicosane	0.5	4.9	MS, RI, O
27	48.83	Methyl margarate	0.6	-	MS, RI, O
28	50.93	Methyl linoleate	9.7	2.5	MS, RI, O
29	51.13	Unidentified	16.0	3.6	MS, RI, O
30	51.28	Methyl elaidate	1.6	-	MS, RI, O
31	51.51	Neophytadiene	18.2	5.3	MS, RI, O
32	51.91	Methyl stearate	3.4	0.7	MS, RI, O
33	52.05	Linoleic acid	0.6	-	MS, RI, O
34	52.24	Oleic acid	1.9	0.8	MS, RI, O
35	52.92	Unidentified	0.5	2.8	MS, RI, O
36	53.11	Unidentified	0.4	-	MS, RI, O
37	53.84	1-Docosene	0.3	2.3	MS, RI, O
38	54.02	Docosane	0.3	3.0	MS, RI, O
39	57.67	Unidentified	0.8	-	MS, RI, O
40	59.43	Unidentified	-	1.4	MS, RI, O
41	59.58	Tetracosane	-	1.6	MS, RI, O
42	63.07	Methyl octacosanoate	0.3	-	MS, RI, O
43	64.18	Heptadecyl heptadecanoate	-	2.1	MS, RI, O
44	74.38	Squalene	1.2	-	MS, RI, O
45	79.68	Unidentified	1.4	-	MS, RI, O
46	79.88	Unidentified	2.9	-	MS, RI, O
47	82.24	α-Tocopherol	1.4	-	MS, RI, O
48	85.41	β-Sitostenone	1.8	-	MS, RI, O
49	87.24	β-Sitosterol	4.5	-	MS, RI, O
50	87.51	Lupeol	1.9	-	MS, RI, O
51	88.57	Unidentified	0.7	-	MS, RI, O
52	89.80	Lupeol acetate	2.3	-	MS, RI, O
		Total	99.3	97.7	
		Unidentified	24.4	10.6	
		Hemiterpenoids/Acids	0.0	0.9	
		Alkanes	3.2	31.2	
		Alkenes	1.0	10.6	
		Alcohols	0.7	6.9	
		Aromatic compounds	1.4	1.1	

No.	RT	Compound[a]	*n*-hexane fraction	Dichloromethane fraction	Identification[b,c]
		Diterpenes	18.2	5.3	
		Triterpenes	1.2	0.0	
		Monoterpenoids	0.2	2.7	
		Diterpenoids	1.4	4.4	
		Triterpenoids	4.2	0.0	
		Steroids	6.3	0.0	
		Fatty acids	5.4	14.6	
		Fatty acid esters	31.6	9.4	

[a]Compound listed according to the elution order of column Equity-5; [b]Retention Index (RI) calculated using a homologous series of *n*-alkanes (C_8-C_{38}) in a capillary column (Equity-5); [c]Identification based on the comparison of mass spectra (MS), retention index (RI) with NIST11, WILEY7, Adams (2017) data libraries, along with http://www.thegoodscentscompany.com/search2.html (accessed on 1 March 2023) (O). Area (%): is the percentage of the area occupied by the compound within the chromatogram; - Not identified

Table S2. SC_{50} values of DPPH scavenging of different extract/fractions of *Grewia bulot* leaves

Concentration (µg/mL)	% DPPH scavenging					
	GBD		GBM		GBH	
	Average	SD	Average	SD	Average	SD
500	95.07	0.91	98.65	1.07	93.64	1.14
100	84.83	1.07	89.90	0.30	41.27	1.44
20	40.59	0.46	75.86	0.68	15.62	1.25
4	19.25	0.54	25.72	0.65	10.51	0.82
SC_{50}[a]	25.51 ± 0.58		9.39 ± 0.90		153.78 ± 7.60	
Concentration (µg/mL)	GBE		GBW		L-Ascorbic acid[b]	
	Average	SD	Average	SD	Average	SD
500	94.52	1.52	96.19	1.32		
100	90.73	0.24	90.35	0.59	92.51	0.23
20	59.47	0.23	33.59	1.23	89.13	1.36
4	21.67	1.48	9.45	1.18	29.20	1.03
0.8					6.61	0.43
SC_{50}	15.42 ± 0.74		31.55 ± 0.79		7.27 ± 0.12	

[a]SC_{50} (concentration that scavenges 50% of DPPH radical); [b]Positive control; GBM: methanol extract; GBH: *n*-hexane, GBD: dichloromethane, GBE: ethyl acetate, and GBW: water fraction, respectively; SD: Standard Deviation

Table S3. Cytotoxic activities of the extract/fractions against four human cancer cell lines

Concentration (µg/mL)	GBH							
	MCF-7		Hep-G2		SK-LU-1		KB	
	% Inhibition	SD	% Inhibition	SD	% Inhibition	SD	% Inhibition	SD
100	50.70	1.97	50.96	1.31	54.05	2.82	58.54	1.44
50	35.92	1.16	27.55	1.21	23.72	2.27	20.29	1.91
25	25.82	1.22	16.82	0.82	14.60	0.98	11.71	0.99
12.5	17.23	1.04	7.99	0.64	7.59	0.65	9.07	0.63
6.25	9.60	0.87	3.58	0.36	4.26	0.15	4.85	0.36
IC_{50}	97.94 ± 6.79		98.27 ± 2.77		93.79 ± 3.52		90.77 ± 1.13	
	GBD							

Concentration (μg/mL)	MCF-7		Hep-G2		SK-LU-1		KB	
	% Inhibition	SD	% Inhibition	SD	% Inhibition	SD	% Inhibition	SD
100	52.71	1.22	43.76	3.40	51.28	2.74	38.87	2.48
50	36.17	1.19	13.05	1.45	29.42	1.06	18.60	1.44
25	26.89	1.68	7.06	0.76	16.96	0.69	8.88	0.57
12.5	15.66	0.93	4.07	0.34	11.17	0.76	4.27	0.29
6.25	8.27	0.67	1.96	0.16	5.32	0.53	2.11	0.22
IC_{50}	90.60 ± 3.49		>100		97.09 ± 5.40		>100	
Concentration (μg/mL)	GBE							
	MCF-7		Hep-G2		SK-LU-1		KB	
	% Inhibition	SD	% Inhibition	SD	% Inhibition	SD	% Inhibition	SD
100	34.91	2.66	24.80	0.93	32.44	2.34	15.30	0.78
50	29.55	1.89	8.43	1.30	16.61	1.80	10.12	0.91
25	20.08	1.06	5.13	0.13	11.37	0.69	6.72	0.81
12.5	12.82	0.97	3.56	0.44	7.89	0.79	3.45	0.34
6.25	7.39	0.38	0.50	0.06	3.35	0.40	1.38	0.20
IC_{50}	>100		>100		>100		>100	
Concentration (μg/mL)	GBM							
	MCF-7		Hep-G2		SK-LU-1		KB	
	% Inhibition	SD	% Inhibition	SD	% Inhibition	SD	% Inhibition	SD
100	44.76	1.93	39.39	1.74	45.10	1.14	23.69	1.73
50	13.26	1.18	12.79	1.22	30.83	1.57	11.23	0.96
25	8.33	0.87	6.72	0.82	18.02	1.05	7.32	0.64
12.5	4.17	0.64	4.31	0.35	9.50	0.68	3.16	0.34
6.25	2.40	0.28	1.52	0.15	4.51	0.38	−2.18	0.22
IC_{50}	>100		>100		>100		>100	
Concentration (μg/mL)	GBW							
	MCF-7		Hep-G2		SK-LU-1		KB	
	% Inhibition	SD	% Inhibition	SD	% Inhibition	SD	% Inhibition	SD
100	14.77	1.26	30.27	2.71	35.37	1.41	26.93	2.57
50	9.15	0.83	15.75	1.01	13.69	0.86	17.24	0.76
25	5.18	0.67	8.32	0.58	8.70	0.32	10.18	0.54
12.5	3.16	0.28	5.21	0.37	4.71	0.30	6.34	0.63
6.25	1.83	0.19	2.28	0.26	2.75	0.29	2.75	0.29
IC_{50}	>100		>100		>100		>100	
Concentration (μg/mL)	Ellipticine							
	MCF-7		Hep-G2		SK-LU-1		KB	
	% Inhibition	SD	% Inhibition	SD	% Inhibition	SD	% Inhibition	SD
10	84.56	1.81	90.71	1.69	95.27	2.14	98.49	2.75
2	72.33	1.28	75.12	1.54	76.18	1.10	80.33	1.06
0.4	48.63	1.12	49.02	0.56	49.16	1.08	51.74	1.22
0.08	21.41	0.92	22.02	0.84	22.42	0.98	22.79	1.39
IC_{50}	0.42 ± 0.02		0.39 ± 0.03		0.45 ± 0.02		0.39 ± 0.01	

[a]Positive control; GBM: methanol extract; GBH: *n*-hexane, GBD: dichloromethane, GBE: ethyl acetate, and GBW: water fraction, respectively; SD: Standard Deviation