

Supporting Information

Terpenes and lignans from the roots of *Solanum melongena* L.

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ABSTRACT

Phytochemical investigation of the roots of *Solanum melongena* L. resulted in the isolation of ten terpenes and sixteen lignans, including a new triterpene saponin, officinoterpenoside E (**1**) and twenty-five known compounds (**2-26**). All compounds were firstly isolated from *S. melongena* except **2**, **13**, **21**, **22**. The structures of these compounds were determined by 1D and 2D NMR spectra referring to the literatures, together with high-resolution mass spectrometric analysis. All compounds were evaluated for the cytotoxicity against three cancer cell lines (HepG2, Hela, and MCF-7) *in vitro*. The results showed that compounds **1**, **6**, **20**, **25** and **26** exhibited moderate cytotoxicity against HepG2, Hela and MCF-7 cells with IC₅₀ values in the range of 16.8±1.7 to 29.1±1.9 μM. Therefore, these terpenoids and lignans may have potential biological activity, and also seemed to be of great chemotaxonomic value for *S. melongena*.

Keywords: Solanaceae, *Solanum*, Natural product, Terpene, Lignan, Cytotoxicity

Table S1 ^{13}C -NMR Data of **2-10** (100 MHz in ^{13}C NMR)

NO.	2 ^b	3 ^b	4 ^a	5 ^a	6 ^a	7 ^a	8 ^a	9 ^b	10 ^b
1	47.8	50.5	42.4	42.7	37.0	37.6	42.5	14.2	13.9
2	69.0	69.5	50.7	50.5	49.9	49.3	43.7	132.2	136.4
3	78.2	78.8	201.2	200.4	62.9	33.8	34.2	128.8	124.9
4	43.8	45.0	127.1	128.0	48.0	26.2	35.4	23.0	22.6
5	48.0	49.2	167.4	164.7	77.8	47.8	51.6	42.0	42.8
6	18.6	68.0	80.0	80.0	119.0	42.4	170.5	72.2	80.0
7	32.9	41.5	136.9	148.4	200.7	41.8	125.8	146.9	144.5
8	39.9	39.8	130.0	131.7	101.4	70.7	201.9	111.3	114.8
9	48.3	49.3	68.6	200.6	213.0	41.8	43.8	75.4	68.1
10	38.5	38.7	23.8	27.6	26.6	49.7	40.6	28.4	23.5
11	23.8	24.2	19.5	19.1	32.5	149.3	152.5		
12	122.6	123.4	23.4	23.5	26.7	108.7	108.4		
13	145.0	144.7	24.5	24.7	30.1	21.6	65.8		
14	42.3	43.2				17.2	21.2		
15	28.4	28.7				64.6	16.1		
16	24.1	24.5							
17	46.8	47.1							
18	42.1	42.5							
19	46.5	46.9							
20	31.0	31.4							
21	34.3	34.7							
22	33.3	33.7							
23	66.5	66.6							
24	14.5	16.4							
25	17.4	19.4							
26	17.6	19.1							
27	26.2	26.7							
28	180.6	180.6							
29	33.3	33.7							
30	23.9	24.2							
1'					98.7			103.5	99.8
2'					75.3			75.2	75.1
3'					78.7			78.8	78.6
4'					71.7			71.8	71.7
5'					78.6			78.5	78.1
6'					63.8			62.8	62.9

^a Measured in CD₃OD^b Measured in C₅D₅N

Table S2 ¹³C-NMR Data of **11-26** (100 MHz in ¹³C NMR)

NO.	11 ^a	12 ^a	13 ^b	14 ^a	15 ^a	16 ^a	17 ^a	18 ^a	19 ^a	20 ^a	21 ^a	22 ^a	23 ^a	24 ^a	25 ^a	26 ^a
1	139.6	135.6	132.1	130.4	130.4	129.1	132.7	133.2	132.3	133.7	133.6	133.7	139.3	138.6	134.2	133.8
2	104.5	104.9	102.7	125.2	112.6	107.8	115.7	115.6	114.8	111.7	111.7	110.6	106.8	113.8	111.8	111.4
3	154.4	154.4	147.1	112.5	148.9	148.9	148.5	148.7	148.6	147.2	147.2	149.2	149.0	149.0	148.7	148.6
4	135.6	139.5	134.2	153.1	153.2	153.2	146.8	146.9	146.1	151.7	148.7	147.9	134.5	146.0	146.9	146.8
5	154.4	154.4	147.1	148.9	115.7	148.9	114.3	114.7	115.7	115.8	115.8	116.3	149.0	116.0	118.3	115.6
6	104.5	104.9	102.7	115.7	125.2	107.8	122.6	123.2	123.4	120.6	120.7	119.9	106.8	123.2	120.8	120.7
7	87.6	87.1	86.1	199.7	199.6	199.4	87.4	84.9	82.8	73.9	74.3	90.6	42.3	48.1	75.1	74.1
8	55.5	55.7	54.3	56.3	56.3	56.6	57.0	56.1	56.5	85.7	88.7	54.3	49.9	48.0	86.2	87.2
9	72.9	73.0	71.8	65.5	65.5	65.4	65.0	64.4	64.5	62.1	62.1	64.5	64.2	62.2	62.1	61.7
1'	133.1	135.6	132.1	129.9	129.3	129.0	132.6	132.3	134.0	155.8	133.5	132.8	130.2	129.0	139.3	136.6
2'	104.8	104.9	102.7	112.7	106.7	106.7	115.5	115.5	111.8	148.9	107.9	122.3	107.8	112.4	112.4	104.0
3'	149.4	154.4	147.1	149.3	149.6	149.6	148.3	148.3	148.2	111.6	154.8	131.2	148.7	147.2	151.3	154.7
4'	136.2	139.5	134.2	147.0	136.0	136.1	146.0	146.2	146.7	131.8	143.3	155.6	138.9	145.3	148.0	138.8
5'	149.4	154.4	147.1	116.6	149.6	149.6	112.3	111.8	115.7	127.2	154.8	146.3	147.7	117.3	115.6	154.7
6'	104.8	104.9	102.7	122.2	106.7	106.7	121.6	121.3	121.0	115.9	107.9	113.9	126.2	134.2	120.2	103.9
7'	87.2	87.1	86.1							192.9	193.0	192.7	33.6	33.6	74.0	89.7
8'	55.7	55.7	54.3										40.9	40.0	56.6	55.0
9'	72.9	73.0	71.8										66.8	65.9	64.3	64.6
1''									65.2						132.0	129.9
2''									15.6						115.6	114.3
3''															148.3	146.1
4''															146.2	152.8
5''															114.5	130.9
6''															123.2	119.9
7''																156.0
8''																127.3
9''																196.1
1'''	105.3	105.3														
2'''	75.7	75.7														
3'''	78.4	78.3														
4'''	71.3	71.3														
5'''	77.8	77.8														
6'''	62.6	62.6														
1''''		105.3														
2''''		75.7														
3''''		78.3														
4''''		71.3														
5''''		77.8														
6''''		62.6														
OCH ₃	57.1	57.1	56.4	56.2	56.8	56.8	56.8	57.1	56.3	56.3	56.4	56.3	56.8	56.3	56.4	56.8
OCH ₃	57.1	57.1	56.4	56.4	56.8	56.8	56.3	56.5	56.1	56.5	56.8	56.7	56.8	56.4	56.4	56.8
OCH ₃	56.8	57.1	56.4		56.8	56.8	56.0	56.4					56.6		56.4	56.6
OCH ₃	56.8	57.1	56.4			56.8							60.1			56.3

^a Measured in CD₃OD^b Measured in CDCl₃

Table S3 Cytotoxic activities of compounds (**1-26**) from the roots of *Solanum melongena* L.

Compound	IC ₅₀ (μM)			Compound	IC ₅₀ (μM)		
	HepG2	Hela	MCF-7		HepG2	Hela	MCF-7
1	16.8 ± 1.7	25.9 ± 2.3	22.8 ± 2.1	15	44.4 ± 3.7	66.7 ± 4.4	61.7 ± 2.0
2	55.1 ± 3.3	37.8 ± 3.6	68.8 ± 4.1	16	53.5 ± 2.9	55.6 ± 3.4	48.8 ± 4.1
3	70.3 ± 4.4	>80	>80	17	>80	69.9 ± 3.7	59.7 ± 2.9
4	>80	>80	62.8 ± 4.5	18	>80	>80	71.2 ± 3.3
5	58.7 ± 1.9	72.8 ± 2.3	>80	19	>80	>80	>80
6	25.5 ± 1.2	28.8 ± 1.9	24.7 ± 2.5	20	19.8 ± 1.7	24.6 ± 2.4	27.8 ± 2.1
7	>80	>80	68.6 ± 2.7	21	38.9 ± 2.8	29.7 ± 1.9	58.8 ± 2.9
8	>80	>80	>80	22	>80	>80	>80
9	42.7 ± 2.3	55.6 ± 3.9	47.8 ± 2.1	23	>80	>80	>80
10	51.6 ± 3.0	55.7 ± 2.4	61.4 ± 2.2	24	>80	>80	>80
11	>80	>80	>80	25	29.1 ± 1.9	22.4 ± 1.3	28.9 ± 1.4
12	>80	>80	>80	26	24.4 ± 2.2	17.8 ± 1.3	26.7 ± 1.6
13	>80	>80	>80	doxorubicin ^a	7.9 ± 1.5	8.8 ± 1.1	6.1 ± 1.9
14	38.9 ± 4.1	46.7 ± 3.2	40.6 ± 1.9				

^a Positive control.

Fig.S1 Key HMBC, ^1H - ^1H COSY and NOESY correlations of compound **1**

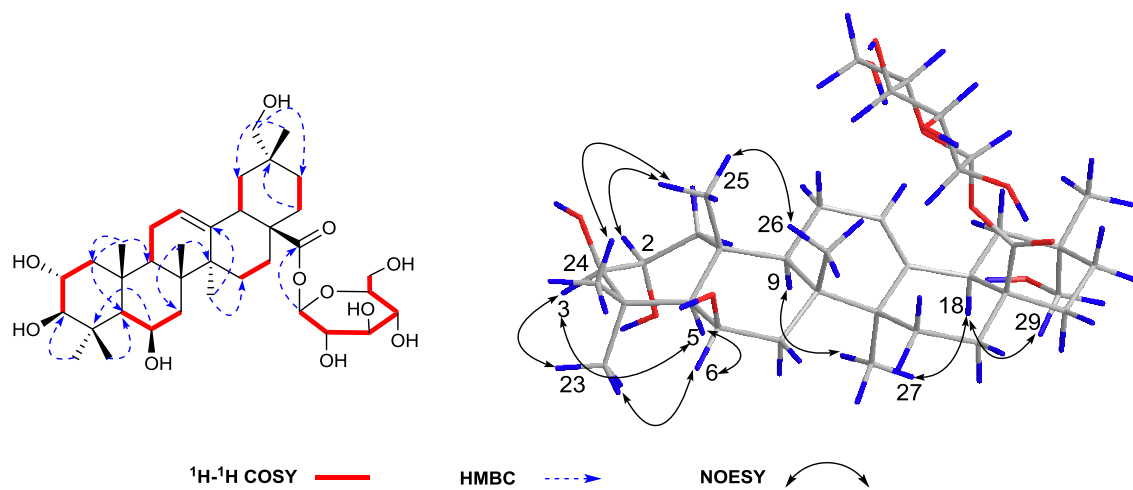


Fig. 2S ^1H NMR spectrum of compound 1

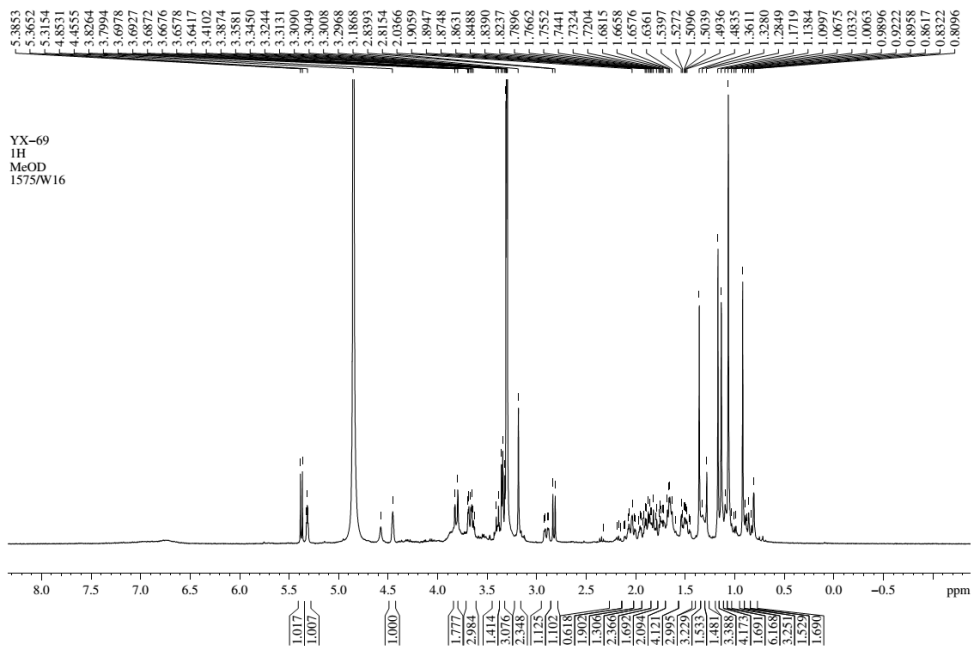


Fig. 3S ^{13}C NMR spectrum of compound 1

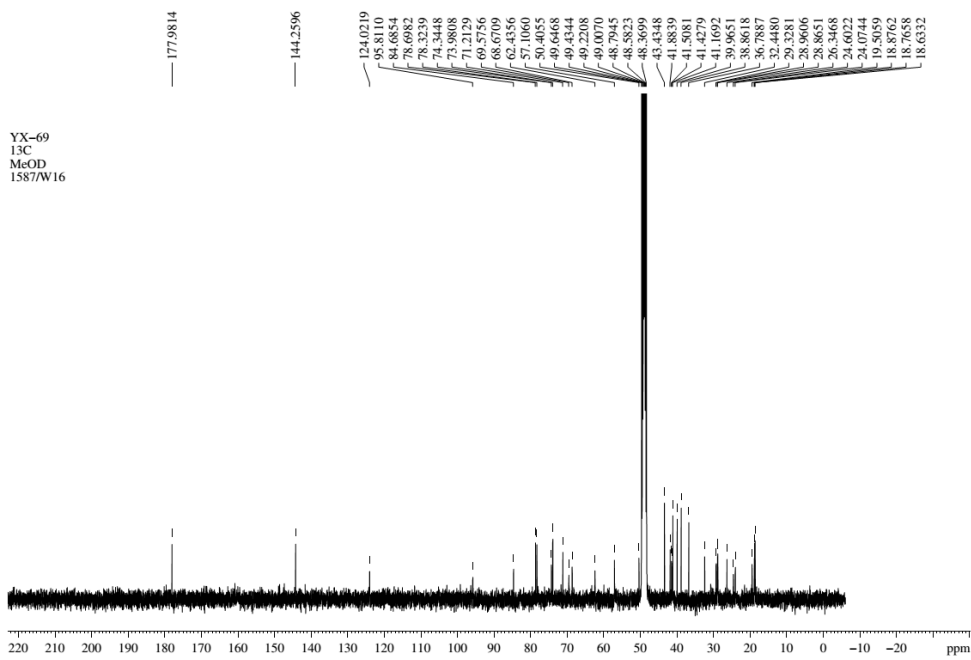


Fig. 4S DEPT-135 spectrum of compound 1

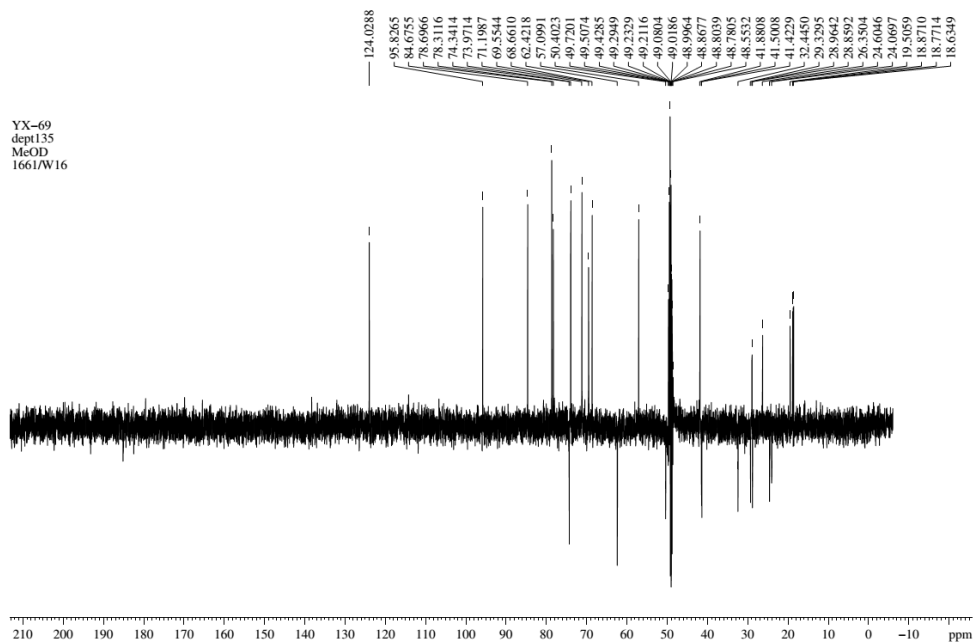


Fig. 5S HSQC spectrum of compound 1

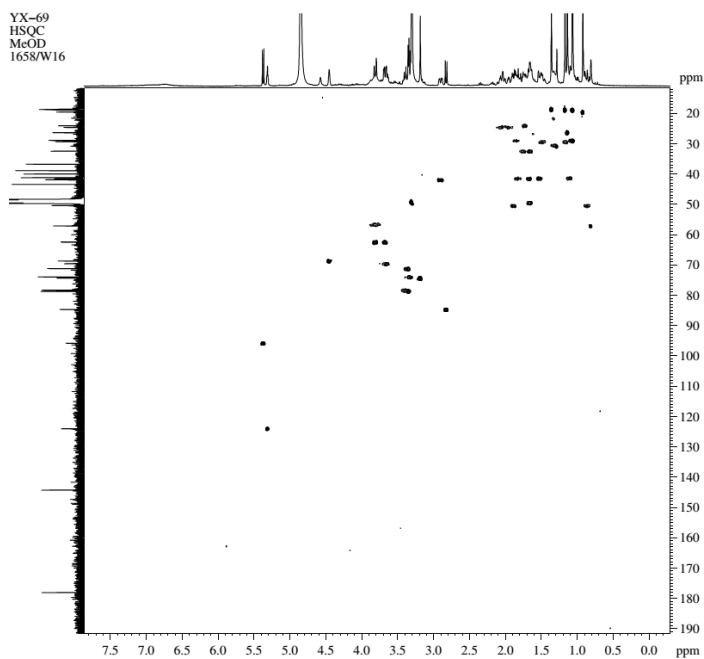


Fig. 6S ^1H - ^1H COSY spectrum of compound **1**

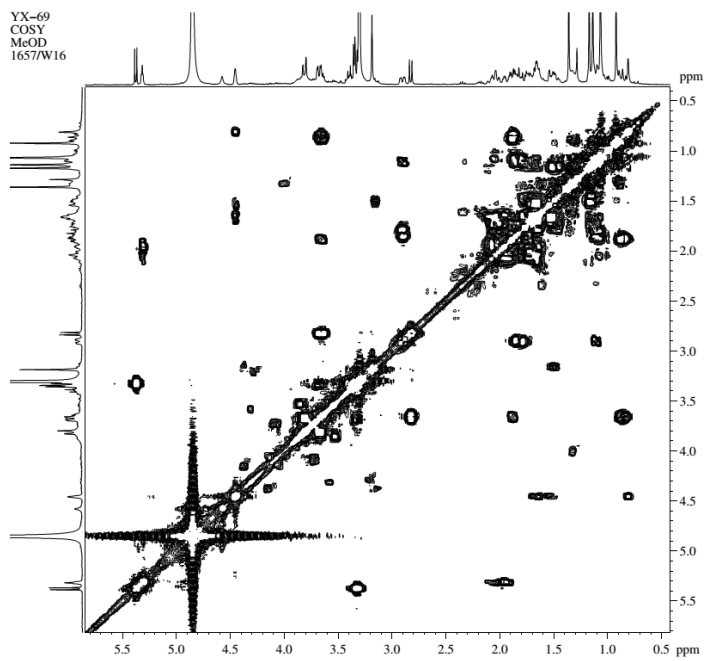


Fig. 7S HMBC spectrum of compound **1**

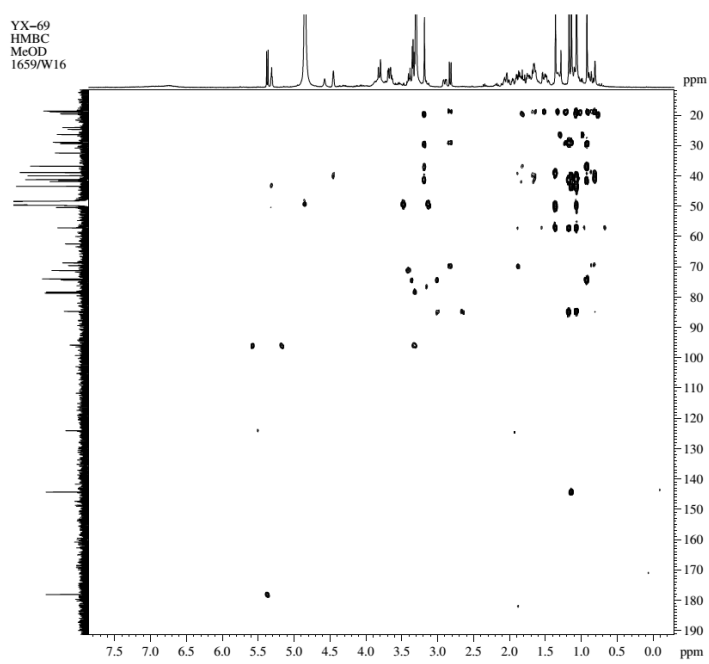


Fig. 8S NOESY spectrum of compound **1**

