

## SUPPLEMENTARY MATERIAL

### Lebbeckoside C, a new triterpenoid saponin from the stem barks of *Albizia lebbeck* inhibits the growth of human glioblastoma cells

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## ABSTRACT

One new acacic acid-type saponin, named lebbeckoside C (**1**), was isolated from the roots of *Albizia lebbeck*. Its structure was established on the basis of extensive analysis of 1D and 2D NMR (<sup>1</sup>H, <sup>13</sup>C NMR, DEPT, COSY, TOCSY, ROESY, HSQC and HMBC) experiments, HRESIMS studies, and by chemical evidence as 3-*O*-[ $\beta$ -D-xylopyranosyl-(1 $\rightarrow$ 2)- $\beta$ -D-fucopyranosyl-(1 $\rightarrow$ 6)-[ $\beta$ -D-glucopyranosyl(1 $\rightarrow$ 2)]- $\beta$ -D-glucopyranosyl]-21-*O*-{(2E,6S)-6-*O*-[(2E,6S)-2,6-dimethyl-6-*O*-( $\beta$ -D-quinovopyranosyl)octa-2,7-dienoyl]-4-*O*-[(2E,6S)-2,6-dimethyl-6-*O*-( $\beta$ -D-quinovopyranosyl)octa-2,7-dienoyl]- $\beta$ -D-quinovopyranosyl}-2,6-dimethylocta-2,7-dienoyl}acic acid 28-*O*-[ $\beta$ -D-quinovopyranosyl-(1 $\rightarrow$ 3)-[ $\alpha$ -L-arabinofuranosyl-(1 $\rightarrow$ 4)]- $\alpha$ -L-rhamnopyranosyl-(1 $\rightarrow$ 2)- $\beta$ -D-glucopyranosyl] ester. The isolated saponin (**1**) displayed significant cytotoxic activity against the human glioblastoma cell line U-87 MG and TG1 stem-like glioma cells isolated from a patient tumor with IC<sub>50</sub> values of 1.69  $\mu$ M and 1.44  $\mu$ M, respectively.

**Keywords:** *Albizia lebbeck*, Mimosaceae, Triterpenoid saponin, Cytotoxic activity, U-87 MG and TG1 stem-like glioma cells.

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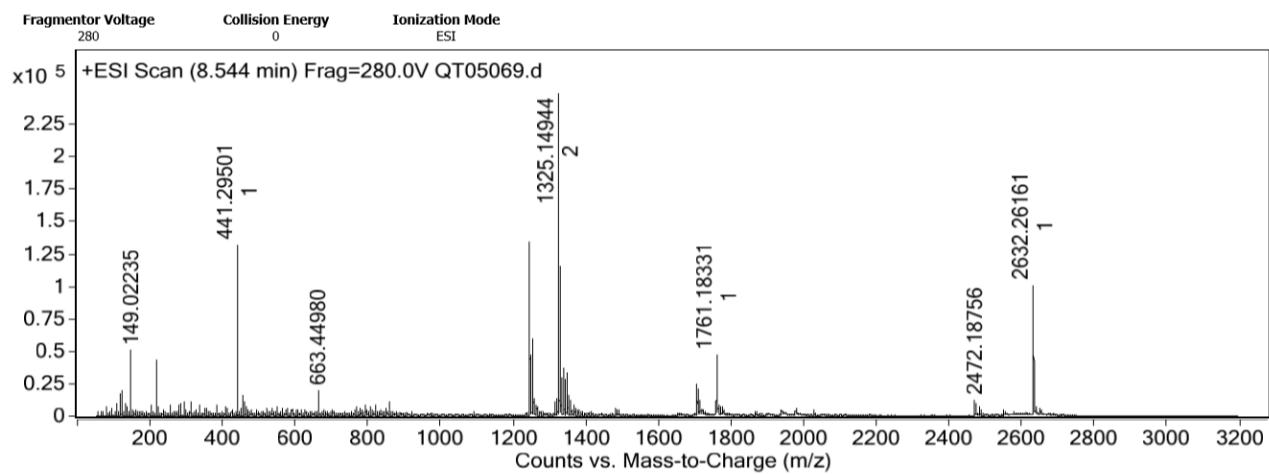
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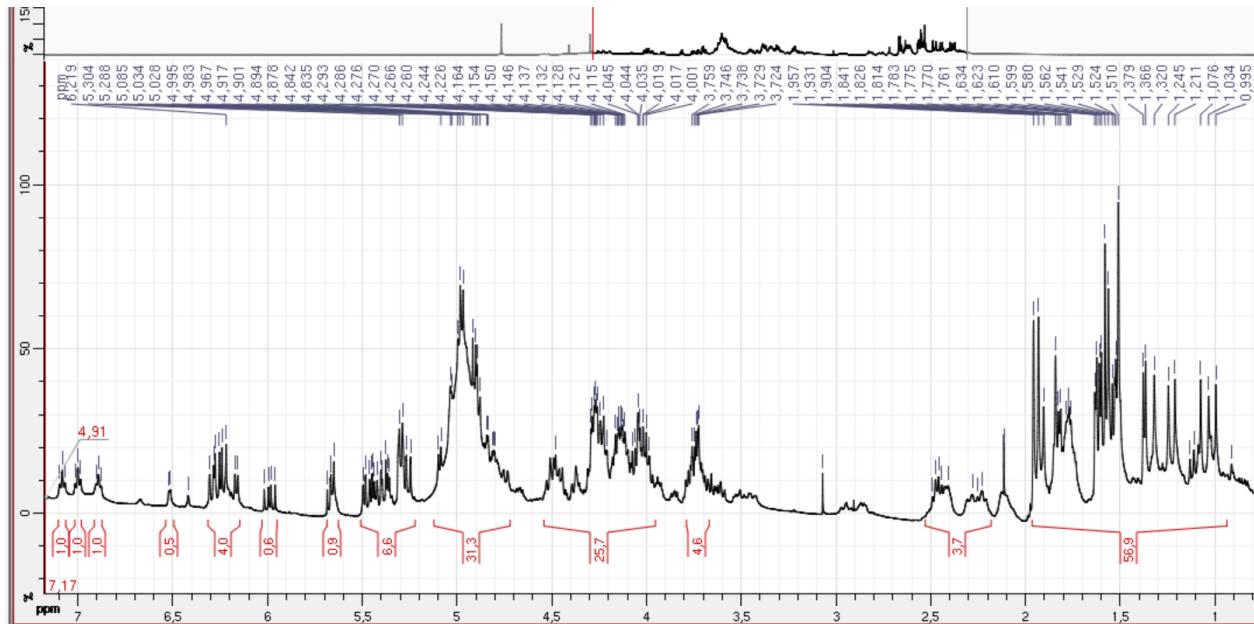
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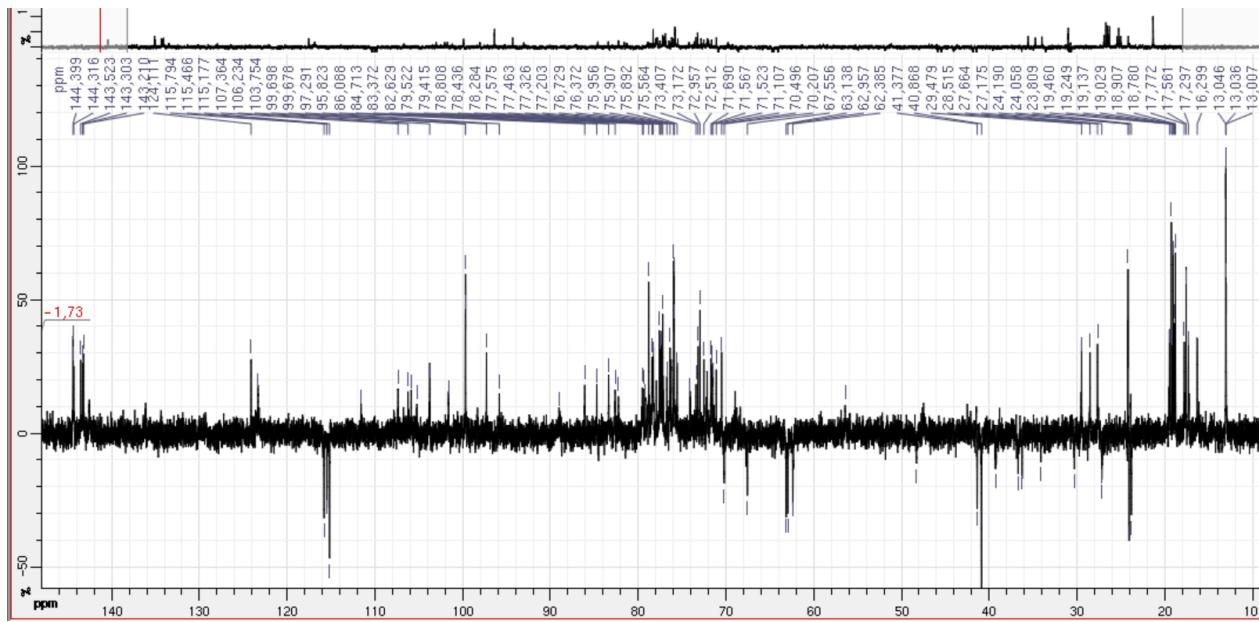
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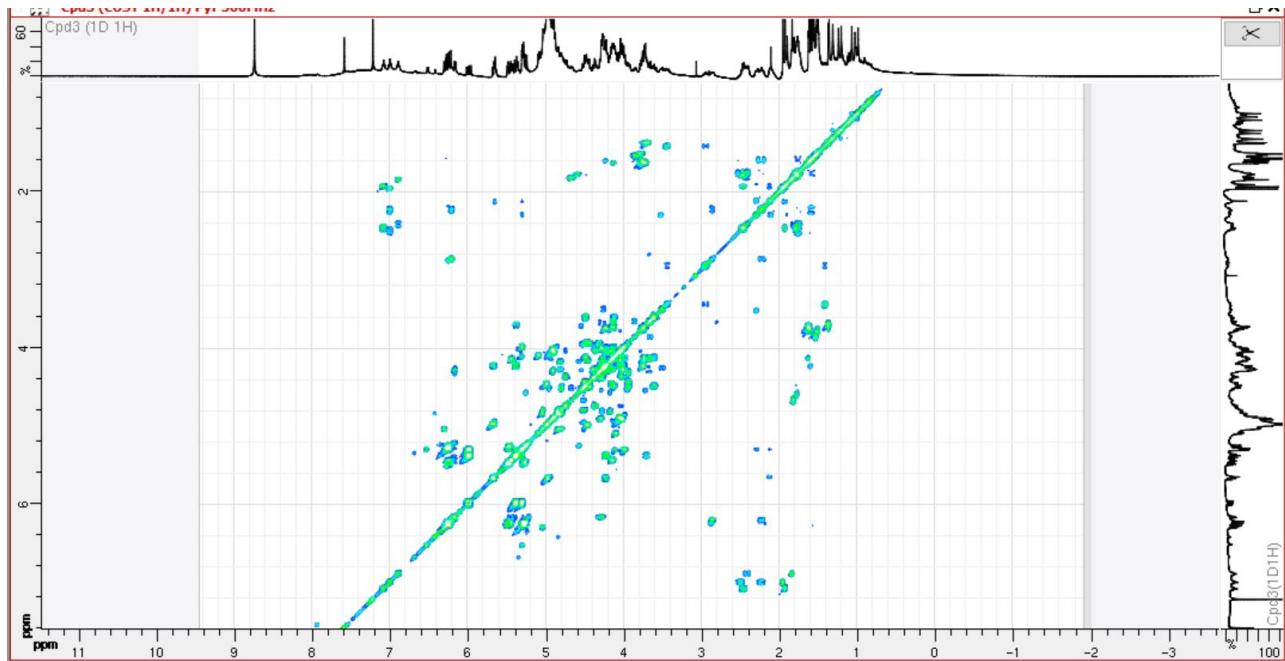
**Figure S1. HRESIMS of compound 1**



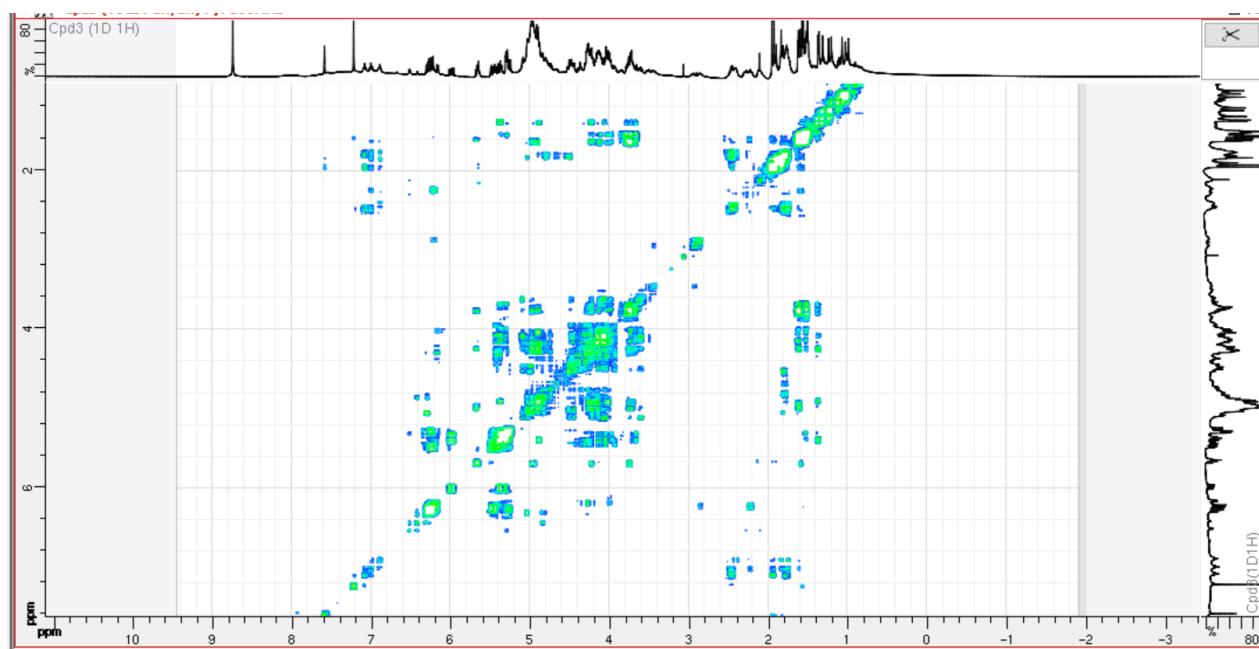
**Figure S2.  $^1\text{H}$  NMR Spectrum of Compound 1 (500 MHz, Pyridine-d<sub>5</sub>)**



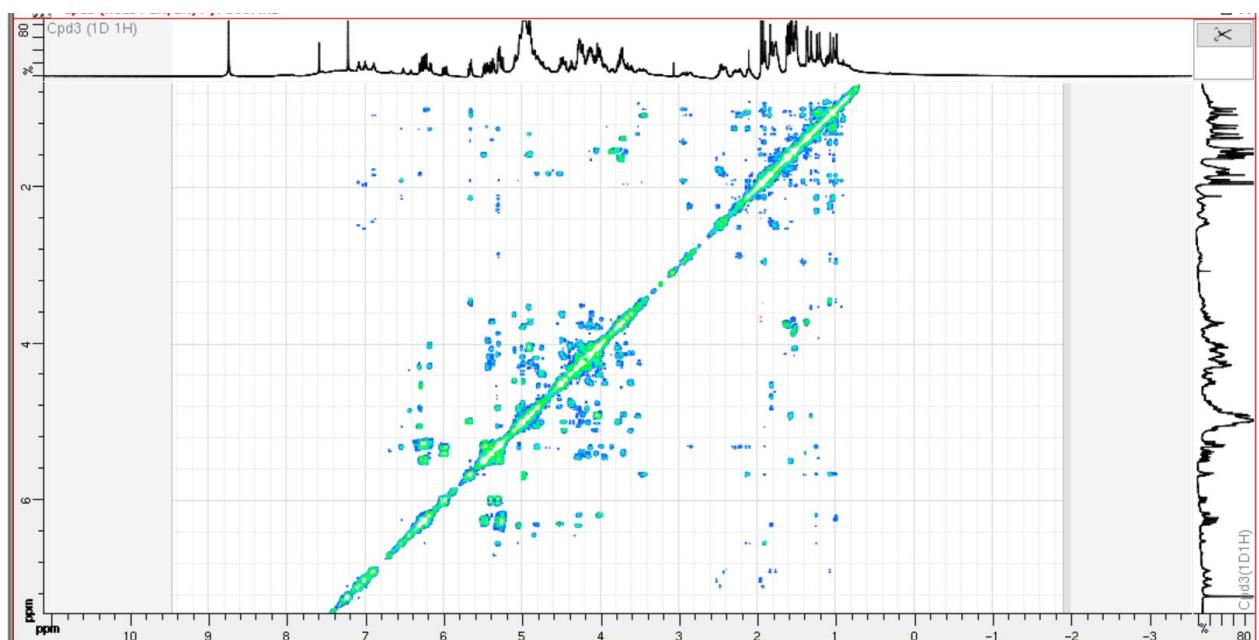
**Figure S3. DEPT 135 Spectrum of Compound 1 (125 MHz, Pyridne-d<sub>5</sub>)**



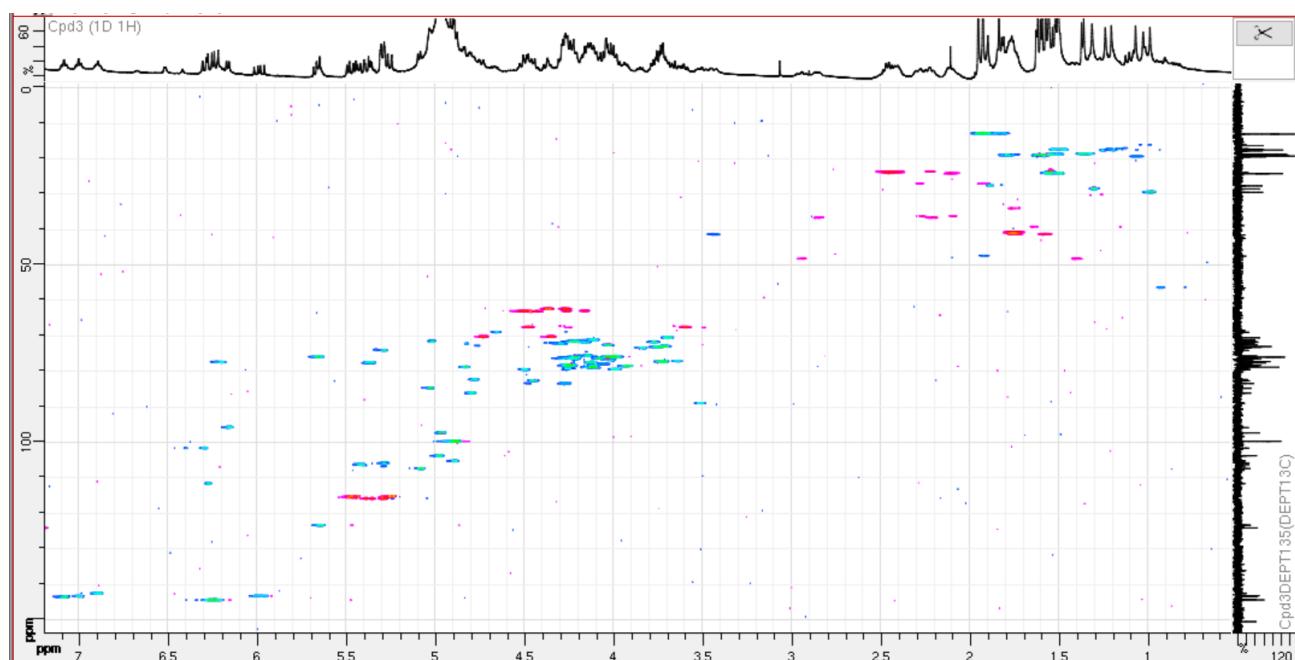
**Figure S4. COSY Spectrum of Compound 1 (500 MHz, Pyridne-d<sub>5</sub>)**



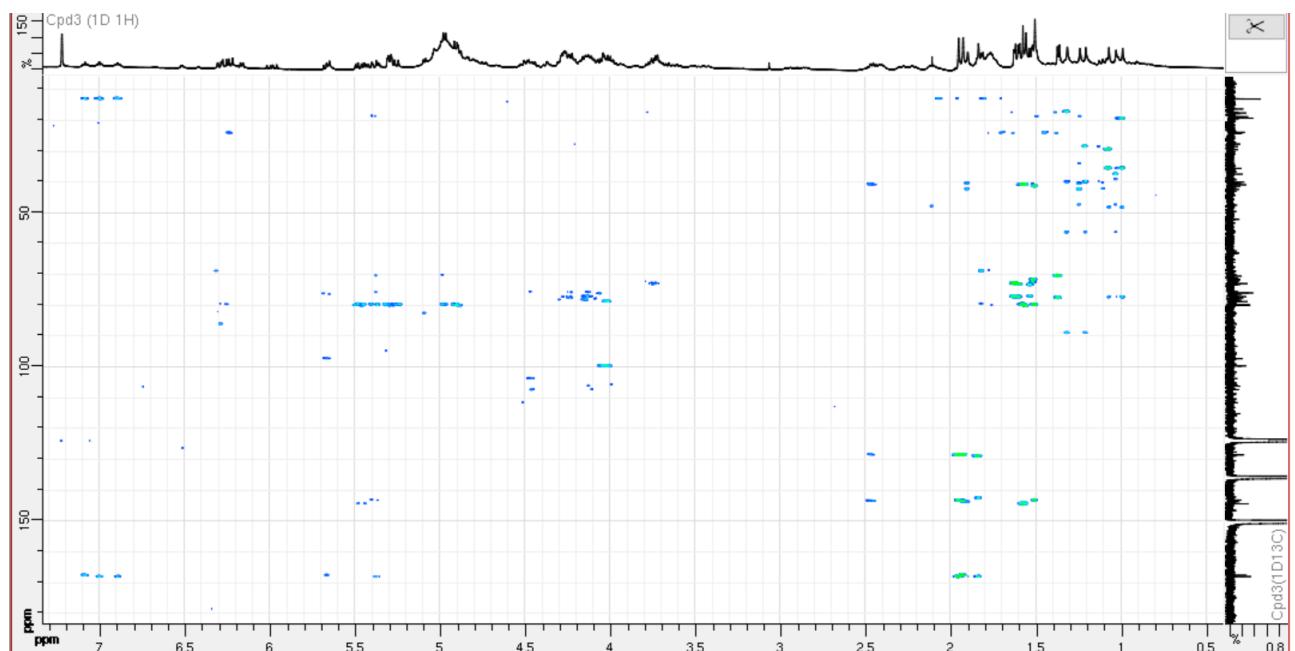
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**Table S1.**  $^1\text{H}$ -NMR (500 MHz) and  $^{13}\text{C}$ -NMR (125 MHz) data of the aglycone part of lebbeckoside C(1) in pyridine-d<sub>5</sub> ( $\delta$  in ppm,  $J$  in Hz)<sup>a</sup>.

Lebbeckoside C (1)							
Position	DEPT	$\delta_{\text{C}}$	$\delta_{\text{H}}$	Position	DEPT	$\delta_{\text{C}}$	$\delta_{\text{H}}$
1	CH <sub>2</sub>	39.2	1.18; 1.66	16	CH	74.0	5.32
2	CH <sub>2</sub>	27.1	1.94; 2.30	17	C	51.9	-
3	CH	88.9	3.52	18	CH	41.4	3.47
4	C	40.3	-	19	CH <sub>2</sub>	48.3	1.42; 2.95
5	CH	56.4	0.94	20	C	35.5	-
6	CH <sub>2</sub>	18.9	1.59; 1.63	21	CH	77.5	5.40
7	CH <sub>2</sub>	34.1	1.78	22	CH <sub>2</sub>	36.7	2.21; 2.87
8	C	40.4	-	23	CH <sub>3</sub>	28.5	1.32 (s)
9	CH	47.4	1.93	24	CH <sub>3</sub>	17.2	1.18 (s)
10	C	37.4	-	25	CH <sub>3</sub>	16.3	1.03 (s)
11	CH <sub>2</sub>	23.8	2.25; 2.47	26	CH <sub>3</sub>	17.5	1.15 (s)
12	CH	123.3	5.68, brs	27	CH <sub>3</sub>	27.6	1.90 (s)
13	C	143.2	-	28	C	174.9	-
14	C	42.4	-	29	CH <sub>3</sub>	29.4	0.99 (s)
15	CH <sub>2</sub>	36.2	2.12; 2.31	30	CH <sub>3</sub>	19.4	1.07 (s)

<sup>a</sup>Assignments were based on the HSQC, HMBC, COSY, TOCSY, NOESY, and DEPT experiments.

Overlapped proton NMR signals are reported without designated multiplicity. nf, not found

**Table S2.**  $^1\text{H}$ -NMR (500MHz) and  $^{13}\text{C}$ -NMR (125 MHz) data of the sugar moieties attached at C-3 and C-28 of compound 1in pyridine-d<sub>5</sub> ( $\delta$  in ppm,  $J$  in Hz)<sup>a</sup>.

Lebbeckoside C (1)					
Position	$\delta_{\text{C}}$	$\delta_{\text{H}}$ ( $J$ in Hz)	Position	$\delta_{\text{C}}$	$\delta_{\text{H}}$ ( $J$ in Hz)
3-O-sugars			28-O-sugars		
Glc I-1	105.2	4.89 d (7.7)	GlcIII-1	95.8	6.16, d (7.6)
2	83.2	4.30	2	76.3	4.31
3	78.4	4.27	3	78.7	4.12
4	71.5	4.23	4	71.4	4.17
5	76.8	4.05	5	79.3	4.02
6	70.0	4.40; 4.77	6	62.3	4.27; 4.39
Fuc- 1	103.7	4.99, d (7.9)	Rha-1	101.6	6.30, brs
2	82.6	4.47	2	71.4	5.03
3	75.5	4.14	3	82.2	4.82
4	72.2	4.06	4	79.5	4.53
5	71.6	3.80	5	68.9	4.67
6	18.5	1.37, d (6.4)	6	18.9	1.82 d (6.4)
Xyl I- 1	107.3	5.09, d (6.6)	Qui-1	105.9	5.29, d (8.0)
2	75.9	4.10	2	75.8	3.98
3	77.8	4.05	3	78.5	3.92
4	71.2	4.14	4	76.2	4.08
5	67.5	3.63; 4.48	5	73.3	3.83
Glc II- 1	106.2	5.43, d (7.7)	6	18.7	1.52 d (6.0)
2	75.6	4.16	Ara <sub>f</sub> -1	111.5	6.29, brs
3	78.8	4.15	2	84.7	5.04
4	72.4	4.17	3	78.7	4.86
5	78.5	3.96	4	86.1	4.83
6	63.1	4.49; 4.30	5	62.8	4.20; 4.27

<sup>a</sup>Assignments were based on the HMBC, HSQC, COSY, TOCSY, NOESY, and DEPT experiments. Overlapped proton NMR signals are reported without designated multiplicity.

**Table S3.**  $^1\text{H}$ -NMR (500 MHz) and  $^{13}\text{C}$ -NMR (125MHz) data of the monoterpene-quinovosyl moiety attached at C-21 of compound **1**in pyridine-d<sub>5</sub> ( $\delta$  in ppm,  $J$  in Hz)<sup>a</sup>.

Position	Lebeckcoside <b>C (1)</b>			
	$\delta_{\text{C}}$	$\delta_{\text{H}}$	$\delta_{\text{C}}$	$\delta_{\text{H}}$
Monoterpene (MT)	Quinovo se (Qui?)			
MT <sub>1</sub> -1	168.1	-	Qui' <sub>1</sub>	
2	128.8	-	1	99.6
3	142.8	6.89, t (7.3)	2	75.8
4	24.0	2.44	3	76.3
5	41.0	1.75	4	77.7
6	79.9	-	5	73.1
7	143.2	6.24, dd (10.3; 17.5)	6	18.8
8	115.7	5.30 d (10.3); 5.40 d (17.5)	Qui' <sub>2</sub>	1.53, d (6.3)
9	13.1	1.84	1	99.6
10	24.1	1.51	2	75.9
MT <sub>2</sub> - 1	167.7	-	3	76.2
2	128.5	-	4	75.9
3	143.3	7.00, t (7.4)	5	73.1
4	23.7	2.26; 2.48	6	18.9
5	40.8	1.79	Qui' <sub>3</sub>	
6	80.0	-	1	97.2
7	144.4	6.28, dd (10.6; 17.0)	2	76.1
8	115.4	5.29 d (10.6); 5.48 d (17.0)	3	76.3
9	13.1	1.96	4	77.2
10	24.2	1.56	5	72.9
MT <sub>3</sub> - 1	167.9	-	6	19.0
2	128.5	-		1.63, d (6.4)
3	143.5	7.08, t (7.4)		
4	23.8	2.26; 2.46		
5	40.8	1.79		
6	79.9	-		
7	144.3	5.98, dd (10.6; 17.0)		
8	115.1	5.25 d (10.6); 5.47 d (17.0)		
9	13.1	1.94		
10	24.3	1.58		

<sup>a</sup>Assignments were based on the HMBC, HSQC, COSY, TOCSY, NOESY, and DEPT experiments. Overlapped proton NMR signals are reported without designated multiplicity.