SUPPLEMENTARY MATERIAL

A new hetero dimeric terpenoid derivative, japonicaside C, from the flower buds of *Lonicera japonica*

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ABSTRACT

A rare hetero dimeric terpenoid derivative, named japonicaside C, together with five known secoiridoid glucosides were isolated from the flower buds of *Lonicera japonica*. The structures of these compounds were established on the basis of spectroscopic analyses. Japonicaside C is the first representative of a novel type of hetero dimeric terpenoid, biogenetically originated from a guaiane-type sesquiterpenoid and a secoiridoid glucoside. Anti-virus activity of the isolated compounds were evaluated *in vitro*.

KEYWORDS

Lonicera japonica, japonicaside C, secoiridoid glucoside, sesquiterpenoid, Anti-virus, RSV

Figure S1 Structure, key HMBC (→) and COSY (→) correlations of compound **1**

Figure S2 Key HMBC (→) and COSY (→) correlations of Part **B** of compound **1**

Figure S3 Key ROESY ($\text{H} \leftrightarrow \text{H}$) correlations of **1**

Tolerance = 5.0 mDa / DBE: min = -1.5, max = 50.0

Element prediction: Off

Number of isotope peaks used for i-FIT = 3

Monoisotopic Mass, Even Electron Ions

187 formula(e) evaluated with 2 results within limits (up to 50 best isotopic matches for each mass)

Elements Used:

Mass	Calc. Mass	mDa	PPM	DBE	Formula	i-FIT	i-FIT Norm	Fit Conf %	C	H	O
625.2866	625.2860	0.6	1.0	9.5	C31 H45 ...	13.1	0.000	100.00	31	45	13
	625.2895	-2.9	-4.6	31.5	C49 H37	29.0	15.867	0.00	49	37	

Figure S4 HR-ESI-Q-TOF-MS spectrum of Compound **1**

Figure S5 ^1H -NMR spectrum of Compound **1**

Figure S6 ¹³C-NMR spectrum of Compound **1**

Figure S7 DEPT-135 spectrum of Compound **1**

Figure S8 ^1H - ^1H COSY spectrum of Compound **1**

Figure S9 HSQC spectrum of Compound **1**

Figure S10 HMBC spectrum of Compound **1**

Figure S10 ROESY spectrum of Compound **1**

Table S1 NMR Spectroscopic Data (CD₃OD) of Compound **1**

Pos.	1		Pos.	1	
	δ_{C}	δ_{H} (<i>J</i> in Hz)		δ_{C}	δ_{H} (<i>J</i> in Hz)
1	97.6	5.54, d (6.6)	1''	47.9	2.97, m
3	152.9	7.41, s	2''	38.5	2.34, dd (18.0, 6.0) 2.08, dd (18.0, 4.8)
4	112.8		3''	211.5	
5	30.2	2.99, d (7.0)	4''	141.9	
		1.86, dt (13.6, 6.9)	5''	174.8	
6	36.2	1.74, m	6''	31.4	2.84, d (12.6) 2.16, d (12.6)
7	96.2	5.07, dd (5.4, 3.6)	7''	74.0	
8	136.2	5.77, ddd (17.4, 10.8, 8.4)	8''	81.5	3.88, dd (12.0, 1.8)
9	45.5	2.62, dd (13.2, 7.2)	9''	33.4	1.56, dt (13.8, 10.8) 1.12, d (13.8)
		5.29, dt (17.4, 1.2)	10''	31.6	2.15, m
10	119.2	5.24, d (10.2)	11''	80.7	
11	171.8		12''	20.6	1.42, s
1'	100.1	4.70, d (7.8)	13''	23.9	1.31, s
2'	74.5	3.19, dd (9.0, 7.8)	14''	21.0	1.05, d (7.2)
3'	78.0	3.37, t (9.0)	15''	8.8	1.68, d (1.8)
4'	71.6	3.27, m			
5'	78.4	3.29, m			
		3.67, dd (12.0, 6.0)			
6'	62.8	3.90, dd (12.0, 1.8)			