## **Supporting Information**

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## A New Iridoid Glycoside from Wine-Processed Corni fructus

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Department	(None Entered)
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#### Scan Graph



Figure S1: UV spectrum of Spectrum of 1 (cornusglucoside I)



Figure S2: IR spectrum of Spectrum of 1 (cornusplucoside I)



Figure S3: HR-ESI-MS Spectrum of 1 (cornusplucoside I)



Figure S4: <sup>1</sup>H-NMR (500 MHz, methanol-*d*<sub>4</sub>) Spectrum of **1** (cornusplucoside I)



Figure S5: <sup>13</sup>C-NMR (125 MHz, methanol-*d*<sub>4</sub>) Spectrum of **1** (cornusplucoside I)



Figure S6: HSQC Spectrum of 1 (cornusplucoside I)



Figure S7: HMBC Spectrum of 1 (cornusplucoside I)



Figure S8: NOESY Spectrum of 1 (cornusplucoside I)

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#### Scan Graph



Figure S9: UV spectrum of Spectrum of 2 (methyl 4-(3',4'-dihydroxyphenyl)-4-oxobutanoate)



Figure S10: IR spectrum of Spectrum of 2 (methyl 4-(3',4'-dihydroxyphenyl)-4-oxobutanoate)



Figure S11: HR-ESI-MS Spectrum of 2 (methyl 4-(3',4'-dihydroxyphenyl)-4-oxobutanoate)



**Figure S12:** <sup>1</sup>H-NMR (500 MHz, methanol-*d*<sub>4</sub>) Spectrum of **2** (methyl 4-(3',4'-dihydroxyphenyl)-4oxobutanoate)



**Figure S13:** <sup>13</sup>C-NMR (125 MHz, methanol-*d*<sub>4</sub>) Spectrum of **2** (methyl 4-(3',4'-dihydroxyphenyl)-4-oxobutanoate)



**Figure S14:** HSQC Spectrum of **2** (methyl 4-(3',4'-dihydroxyphenyl)-4-oxobutanoate)



Figure S15: H<sup>1</sup>-H<sup>1</sup> COSY Spectrum of 2 (methyl 4-(3',4'-dihydroxyphenyl)-4-oxobutanoate)



**Figure S16:** HMBC Spectrum of **2** (methyl 4-(3',4'-dihydroxyphenyl)-4-oxobutanoate)



Figure S17: NOESY Spectrum of 2 (methyl 4-(3',4'-dihydroxyphenyl)-4-oxobutanoate)

	2		
Position	$\delta_{ m H}$	$\delta_{ m C}$	LIT $\delta_{\mathrm{H}}^{[16]}$
1		199.1	
2	3.25 (2H, t, 6.2)	33.8	3.25 (2H, t, 6.4)
3	2.67 (2H, t, 6.2)	29.1	2.67 (2H, t, 6.4)
4		175.4	
5	3.67 (3H, s)	52.2	3.67 (3H, s)
1'		130.2	
2'	7.42 (1H, s)	115.8	7.42 (1H, d, 2.1)
3'		146.5	
4'		152.3	
5'	6.83 (1H, d, 8.0)	115.9	6.83 (1H, d, 8.3)
6'	7.45 (1H, d, 8.0)	122.9	7.45 (1H, dd, 8.2, 2.1)

 Table 1. <sup>1</sup>H and <sup>13</sup>C NMR spectra data (CD<sub>3</sub>OD, 500/125 MHz) for compounds 2 and the <sup>1</sup>H NMR in literature .



**Figure S18:** Cell viabilities of RAW 264.7 cells in present of compounds 1–4. \* P<0.05, \*\* P<0.001, compared with the control group.

### S1 :New Compounds Search Eeport of SciFinder



Candidates Selected Stereo in answer structure

Explore results Answer set 4 created with 3 answers from REGISTRY

October 28, 2021 9:57 PM

Explore substances by similarity: structure initiated, resulting in 9 candidates

Query



Explore complete

Candidates Selected ≥ 99 (most similar) 95-98

Explore results Answer set 6 created with 31 answers from REGISTRY



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