## SUPPORTING INFORMATION

## Dereplication-guided Isolation of New Phenylpropanoidsubstituted Diglycosides from *Cistanche salsa* and Their Inhibitory Activity on NO Production in Macrophage

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## Figure S 1- 1. The HRESIMS of **5.**



Formula (M)		Ion Formula	Mass (MFG)	m/z (Calc)	Diff (ppm)
	C28 H39 Na O14	C28 H39 Na2 O14	622.2238	645.213	-2.62
	C30 H38 O14	C30 H38 Na O14	622.2262	645.2154	1.25
	C46 H31 Na O	C46 H31 Na2 O	622.2273	645.2165	3.02
	C21 H43 Na O19	C21 H43 Na2 O19	622.2296	645.2188	6.82
	C48 H30 O	C48 H30 Na O	622.2297	645.2189	6.89

Figure S 1- 2. The <sup>1</sup>H NMR (800 MHz) spectrum of 5 in DMSO- $d_6$ 



Figure S 1- 3 The  ${}^{13}$ C NMR (200 MHz) spectrum of 5 in DMSO- $d_6$ 





**Figure S 1- 5.** The COSY spectrum of **5** in DMSO- $d_6$ 



**Figure S 1- 6.** The HMBC spectrum of **5** in DMSO- $d_6$ 



Figure S 1- 7. The NOESY spectrum of **5** in DMSO-*d*<sub>6</sub>



Figure S 1- 8. The UV spectrum of **5** 





<b>Counts vs</b>	Mass-to-Charge	(m/z)
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	Formula (M)	Ion Formula	Mass (MFG)	m/z (Calc)	Diff (ppm)
	C24 H37 Na O13	C24 H37 Na2 O13	556.2132	579.2024	-5.38
•	C26 H36 O13	C26 H36 Na O13	556.2156	579.2048	-1.06
	C42 H29 Na	C42 H29 Na2	556.2167	579.2059	0.93
	C44 H28	C44 H28 Na	556.2191	579.2083	5.25

Figure S 2- 2. The <sup>1</sup>H NMR (500 MHz) spectrum of **6** in DMSO- $d_6$ 



Figure S 2- 3. The  ${}^{13}$ C NMR (125 MHz) spectrum of **6** in DMSO- $d_6$ 





Figure S 2- 4. The HSQC spectrum of 6 in DMSO-*d*<sub>6</sub>



Figure S 2- 5. The COSY spectrum of 6 in DMSO-*d*<sub>6</sub>



**Figure S 2- 6.** The HMBC spectrum of **6** in DMSO- $d_6$ 

Figure S 2- 7. The UV spectrum of 6



Figure S 3- 1. The HRESIMS of **12**.



Formula (M)		Ion Formula	Mass (MFG)	m/z (Calc)	Diff (ppm)
	C24 H39 Na O13	C24 H39 Na2 O13	558.2288	581.2181	-5.81
•	C26 H38 O13	C26 H38 Na O13	558.2312	581.2205	-1.5
	C42 H31 Na	C42 H31 Na2	558.2323	581.2216	0.48
	C44 H30	C44 H30 Na	558.2348	581.224	4.79

Figure S 3- 2. The <sup>1</sup>H NMR (800 MHz) spectrum of **12** in DMSO- $d_6$ 



## Figure S 3- 3. The ${}^{13}$ C NMR (200 MHz) spectrum of 12 in DMSO- $d_6$





Figure S 3- 4. The HSQC spectrum of 12 in DMSO-*d*<sub>6</sub>





Figure S 3- 6. The HMBC spectrum of 12 in DMSO-*d*<sub>6</sub>

Figure S 3-7. The UV spectrum of 12





Formula (M)		Ion Formula	Mass (MFG)	m/z (Calc)	Diff (ppm) /
	C29 H39 Na O14	C29 H39 Na2 O14	634.2238	657.213	-2.73
•	C31 H38 O14	C31 H38 Na O14	634.2262	657.2154	1.07
	C47 H31 Na O	C47 H31 Na2 O	634.2273	657.2165	2.81
	C22 H43 Na O19	C22 H43 Na2 O19	634.2296	657.2188	6.54
	C49 H30 O	C49 H30 Na O	634.2297	657.2189	6.6

Figure S 4- 2. The <sup>1</sup>H NMR (300 MHz) spectrum of 17 in DMSO- $d_6$ 





Figure S 4- 3. The  ${}^{13}$ C NMR (75 MHz) spectrum of 17 in DMSO- $d_6$ 



Figure S 4- 4. The HSQC spectrum of 17 in DMSO-*d*<sub>6</sub>



Figure S 4- 5. The COSY spectrum of 17 in DMSO-*d*<sub>6</sub>

Figure S 4- 6. The HMBC spectrum of 17 in DMSO- $d_6$ 



Figure S 4- 7. The UV spectrum of 17



Figure S 5-1. The HRESIMS of **18**.



	Formula (M)	Ion Formula	Mass (MFG)	m/z (Calc)	Diff (ppm)
	C29 H39 Na O14	C29 H39 Na2 O14	634.2238	657.213	-5.72
Þ	C31 H38 O14	C31 H38 Na O14	634.2262	657.2154	-1.93
	C47 H31 Na O	C47 H31 Na2 O	634.2273	657.2165	-0.19
	C22 H43 Na O19	C22 H43 Na2 O19	634.2296	657.2188	3.54
	C49 H30 O	C49 H30 Na O	634.2297	657.2189	3.61
	C24 H42 O19	C24 H42 Na O19	634.232	657.2213	7.33

Figure S 5- 2. The <sup>1</sup>H NMR (800 MHz) spectrum of 18 in DMSO- $d_6$ 



Figure S 5- 3. The  ${}^{13}$ C NMR (200 MHz) spectrum of 18 in DMSO- $d_6$ 



Figure S 5- 4. The HSQC NMR spectrum of **18** in DMSO-*d*<sub>6</sub>





Figure S 5- 5. The COSY NMR spectrum of 18 in DMSO-*d*<sub>6</sub>







Figure S 5-7. The UV spectrum of 18



**Figure S6- 1.** Effects of compounds on the NO production and cell viability of RAW 264.7 cells.

(A) Cells cultured in phenol red- and serum-free media were pretreated with each compound for 30 min and then stimulated with 500 ng/ml final concentration LPS for 24 h. In the culture medium, NO production was measured based on the Griess reaction, as described in the Materials and Methods section. \* significant difference from LPS cells, p < 0.05. (B) Cells grown in serum-free media were treated with 50 µM of each compound for 24 h, and cell viability was assessed by MTT assay, as described in the Materials and Methods section. Results of independent experiments were averaged and are shown as the percentage of cell viability compared with the viability of normal control cells. Results of independent experiments were averaged and are shown as the percentage of cell viability compared with the viability of solvent control cells.

Figure S6- 2. Dose-response curves of compounds 5, 11, 13 and 18

