

SUPPLEMENTARY MATERIAL

A new pentacyclic triterpenoid from the leaves of *Rhododendron dauricum* L. with inhibition of NO production in LPS-induced RAW 264.7 cells

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Abstract: A new pentacyclic triterpenoid, 3-oxo-urs-11,13(18)-dien-28-oic acid (**1**), along with twelve known triterpenoids, α -amyrin (**2**), 19 α -hydroxy- α -amyrin (**3**), triptohypol E (**4**), uvaol (**5**), 2 α ,3 α -dihydroxyurs-11-en-13 β ,28-olide (**6**), 3 β -hydroxyurs-11-en-13 β ,28-olide (**7**), ursolic acid (**8**), asiatic acid (**9**), oleanolic acid (**10**), aegiceradienol (**11**), obtusalin (**12**) and betulinic acid (**13**) were isolated from the leaves of *Rhododendron dauricum* L. Their structures were established from spectroscopic data and comparison with reported values. Among them, compounds **3**, **4**, **6**, **7** and **11** were isolated from the Ericaceae family for the first time. Compounds **2**, **5**, **9**, **12** and **13** were obtained from *R. dauricum* for the first time. Additionally, compounds **6**, **10** and **11** significantly inhibited the levels of NO in LPS-stimulated RAW 264.7 cells at 3 μ M.

Keywords: *Rhododendron dauricum* L.; Ericaceae; triterpenoid; NO

Structure elucidation of isolated compounds 2-13

The known compounds **2–13** were identified as α -amyrin (**2**) (Li et al. 2016), 19 α -hydroxy- α -amyrin (**3**) (Akbar et al. 2002), triptohypol E (**4**) (Fujita et al. 2000), uvaol (**5**) (Greve et al. 2017), 2 α ,3 α -dihydroxyurs-11-en-13 β ,28-olide (**6**) (Ikuta et al. 2003), 3 β -hydroxyurs-11-en-13 β ,28-olide (**7**) (Abdel-Monem et al. 2015), ursolic acid (**8**) (Liu et al. 2016), asiatic acid (**9**) (Liu et al. 2006), oleanolic acid(**10**) (Liao et al. 2014), aegiceradienol (**11**) (Huang et al. 1999), obtusalin (**12**) (Xu et al. 2012), betulinic acid (**13**) (Yili et al. 2009).

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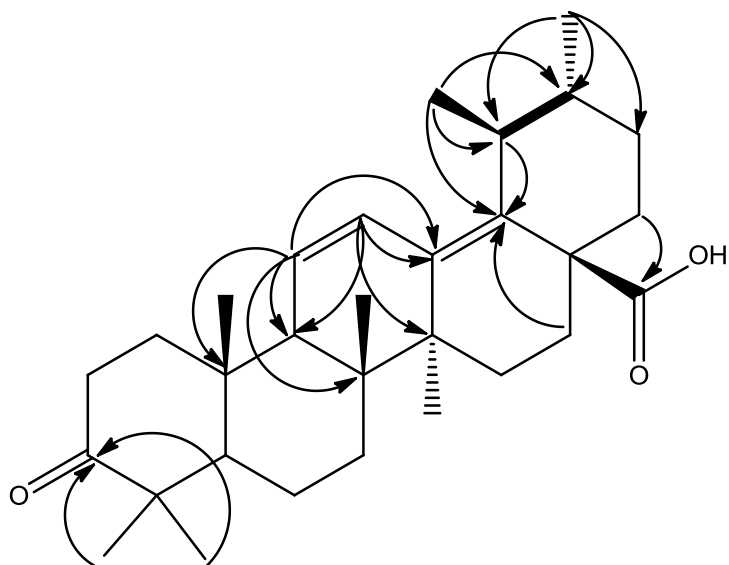


Figure S1. Key HMBC (H→C) and ¹H-¹H COSY (—) correlations of compound **1**.

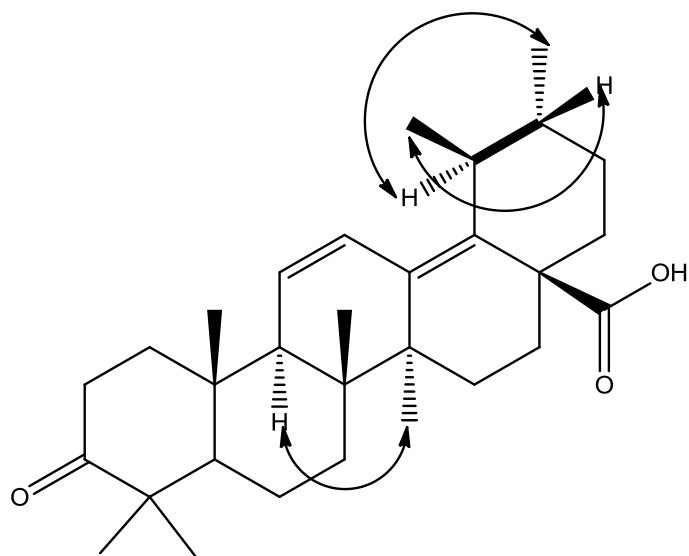


Figure S2. Key NOESY correlations of compound **1**.

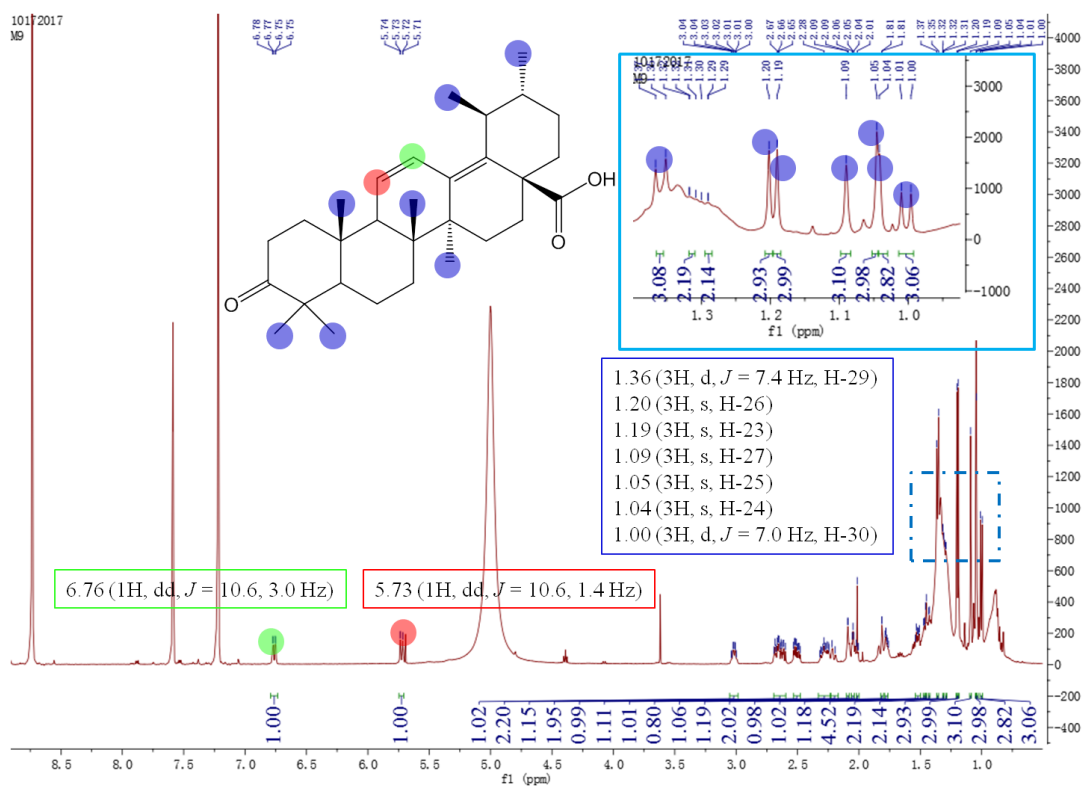


Figure S3. ¹H NMR spectrum of compound **1** in pyridine-*d*₅ (500 MHz)

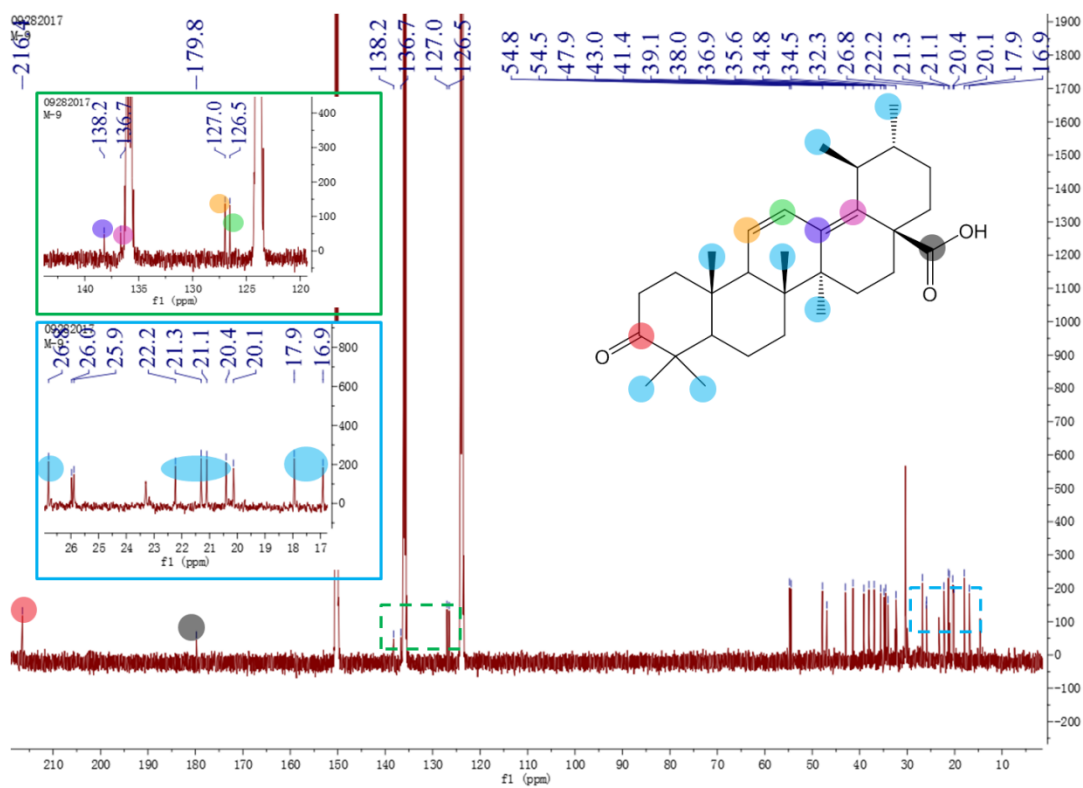


Figure S4. ¹³C NMR spectrum of compound **1** in pyridine-*d*₅ (125 MHz).

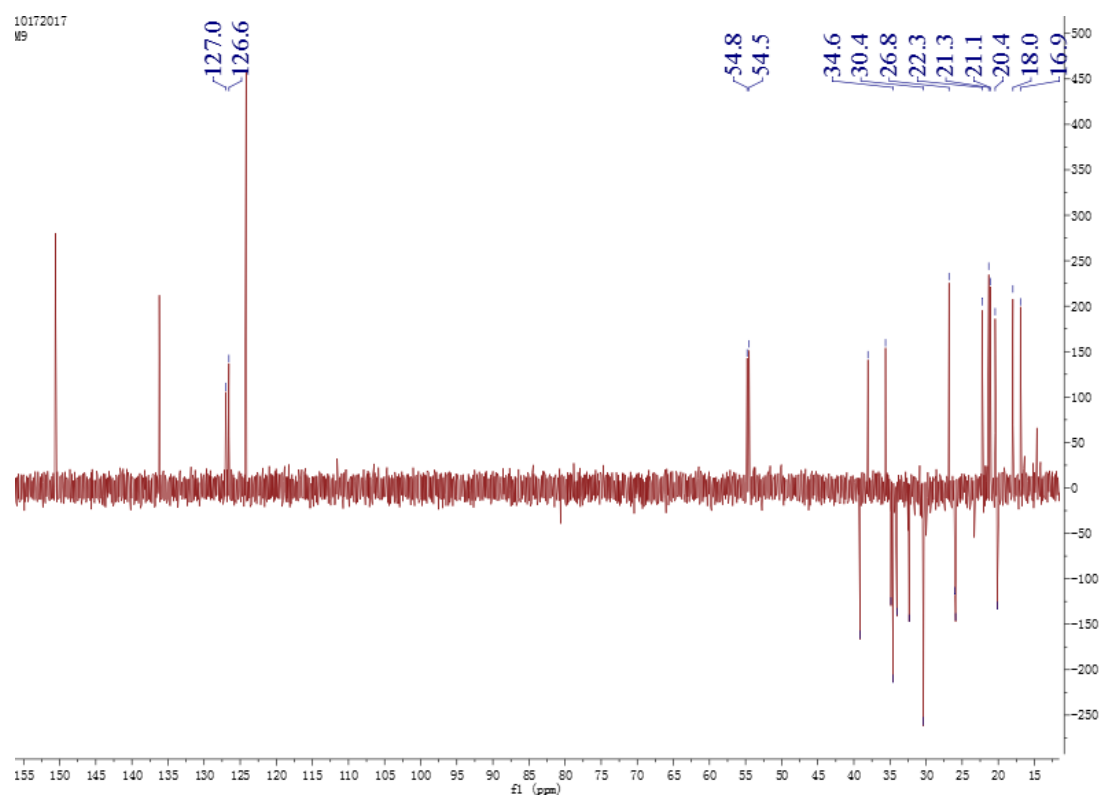


Figure S5. DEPT-135 spectrum of compound **1** in pyridine- d_5 .

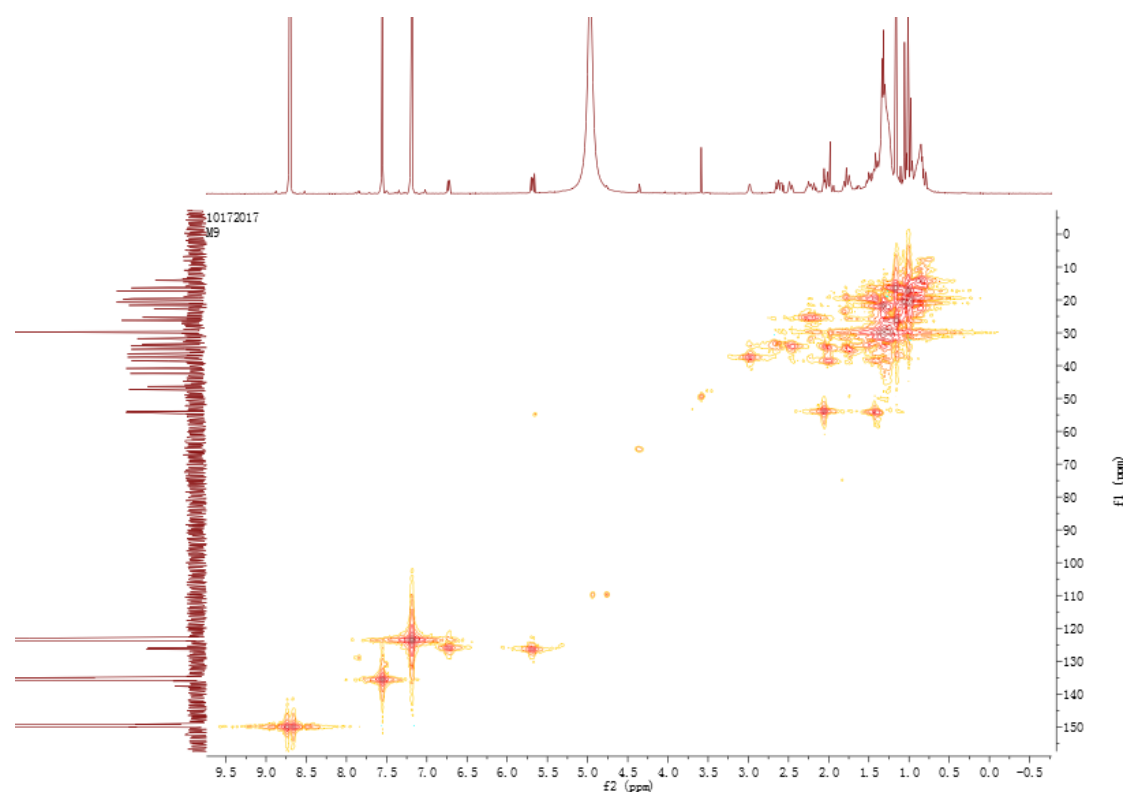
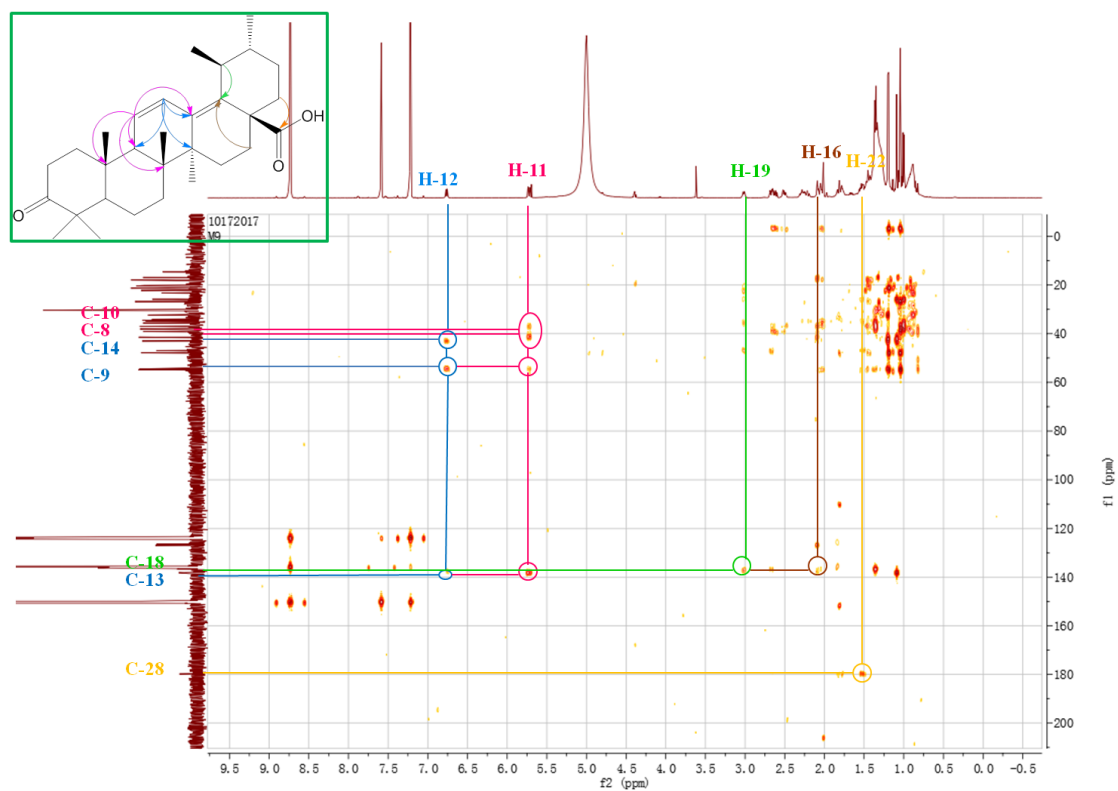
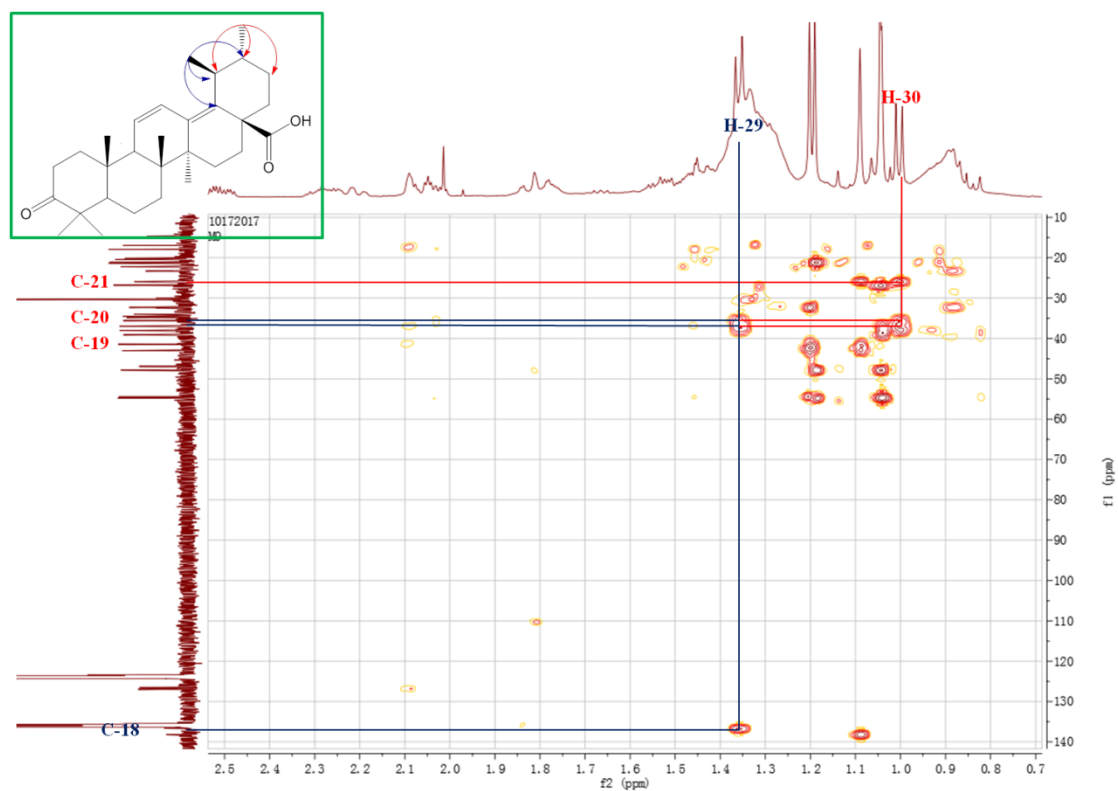


Figure S6. HMQC spectrum of compound **1** in pyridine- d_5 .



500M-HMBC



500M-HMBC

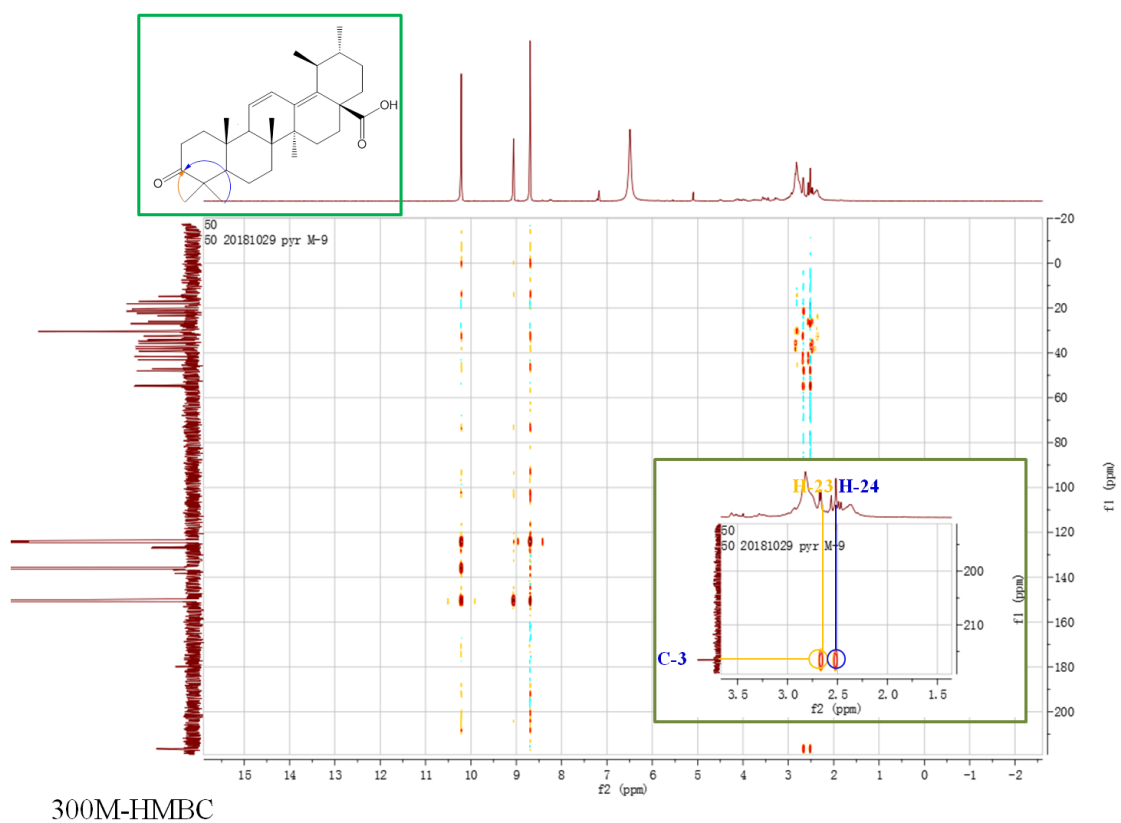
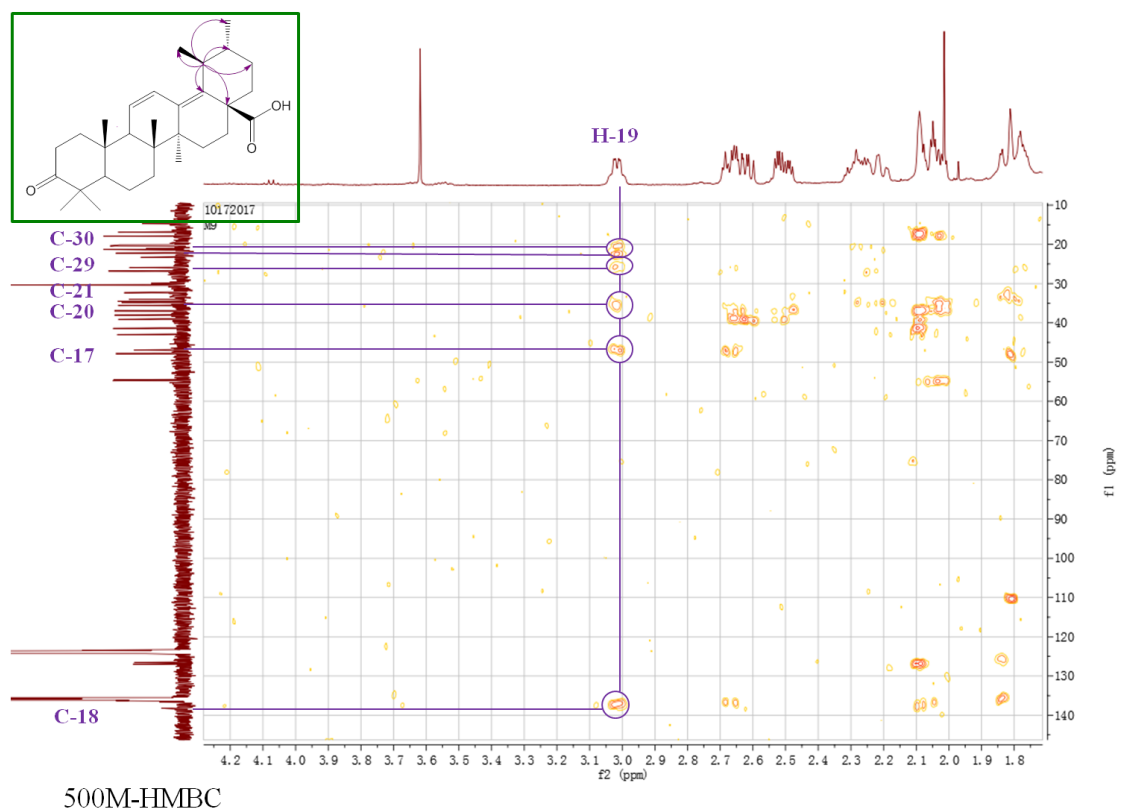


Figure S7. HMBC spectrum of compound **1** in pyridine- d_5 .

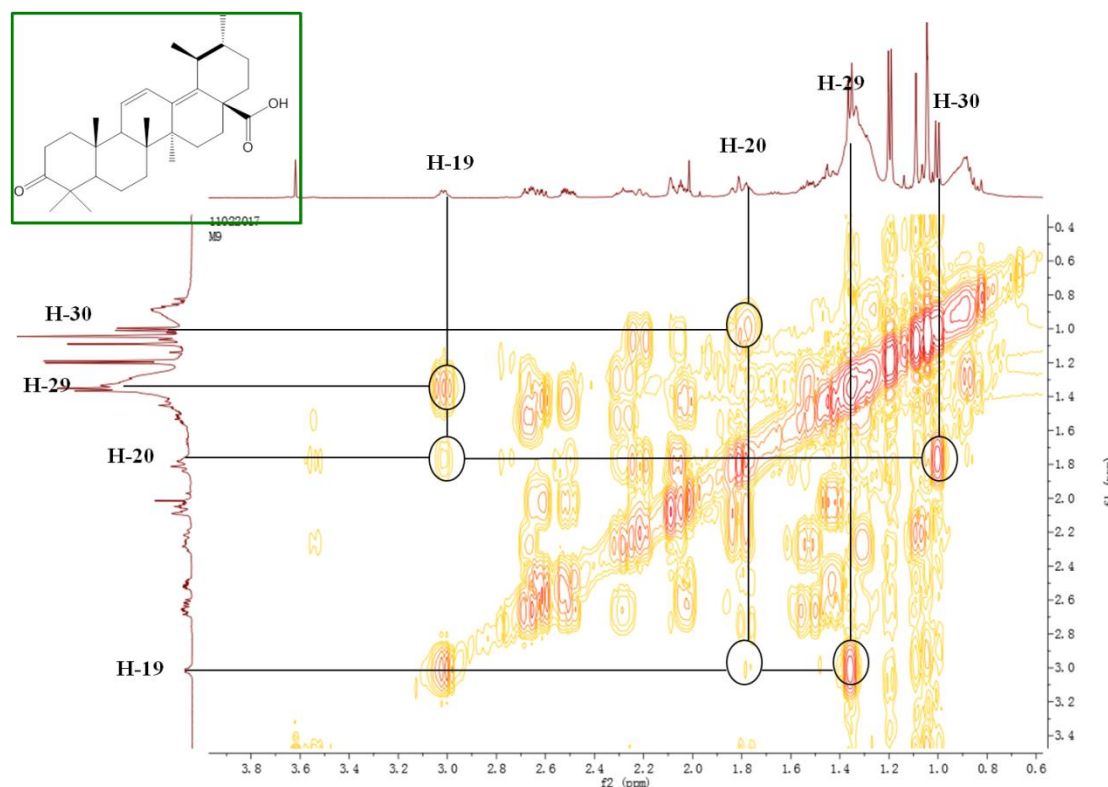


Figure S8. COSY spectrum of compound **1** in pyridine- d_5 .

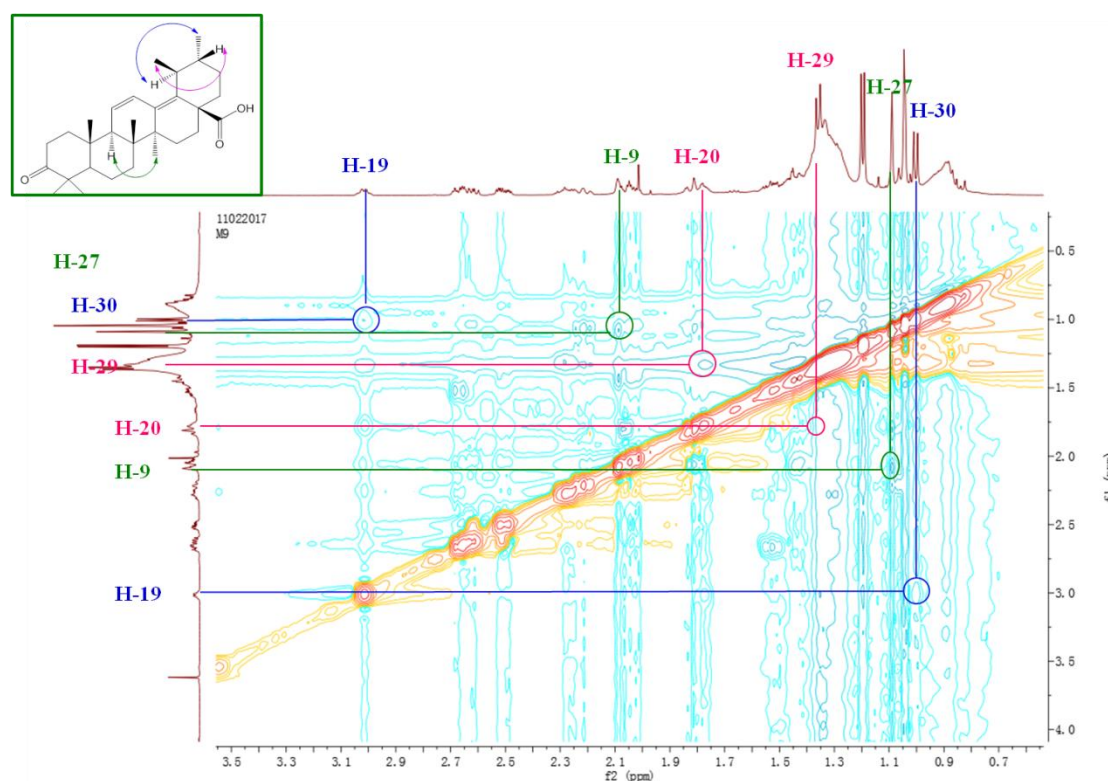


Figure S9. NOESY spectrum of compound **1** in pyridine- d_5 .

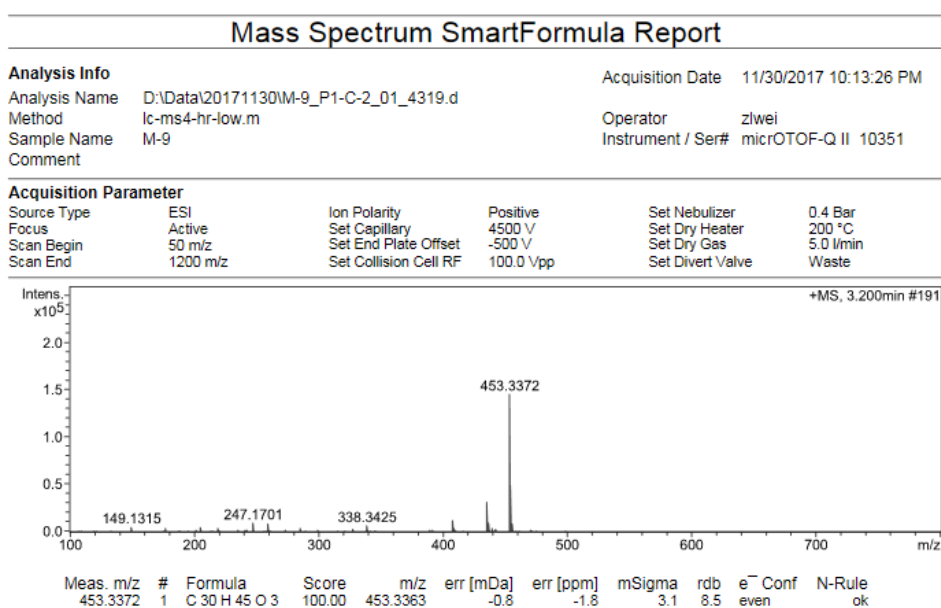


Figure S10. HR-ESI-MS spectrum of compound **1**.

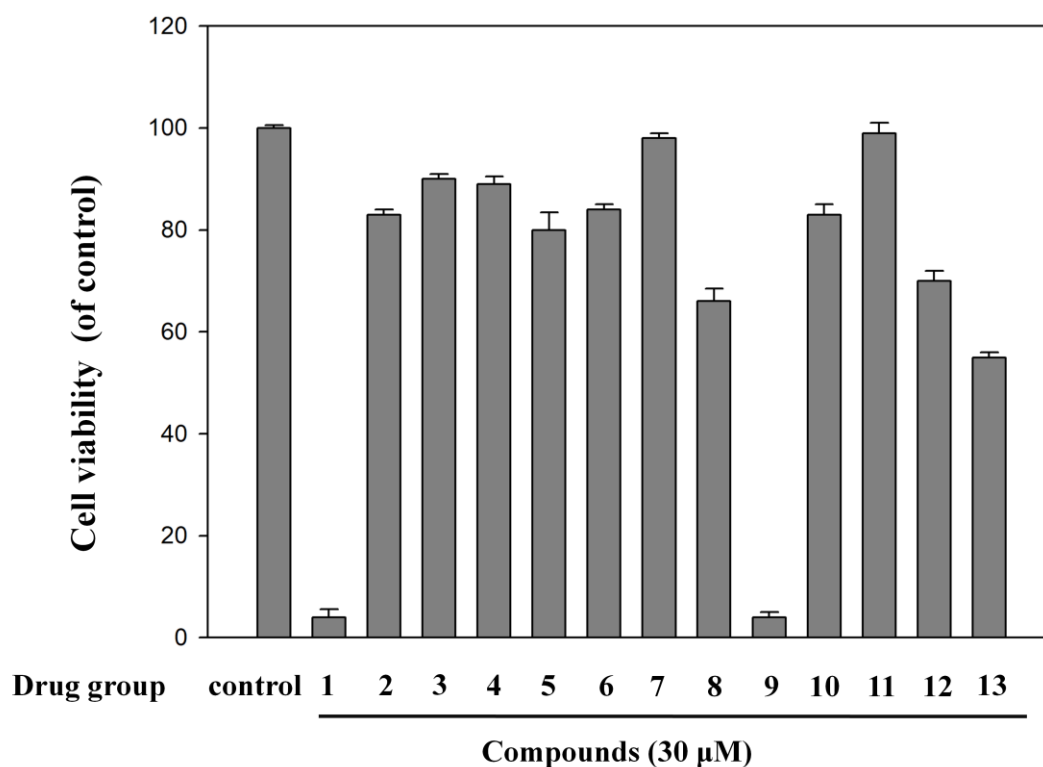


Figure S11. Cell viability of compounds **1–13** in LPS-stimulated RAW 264.7 cells.

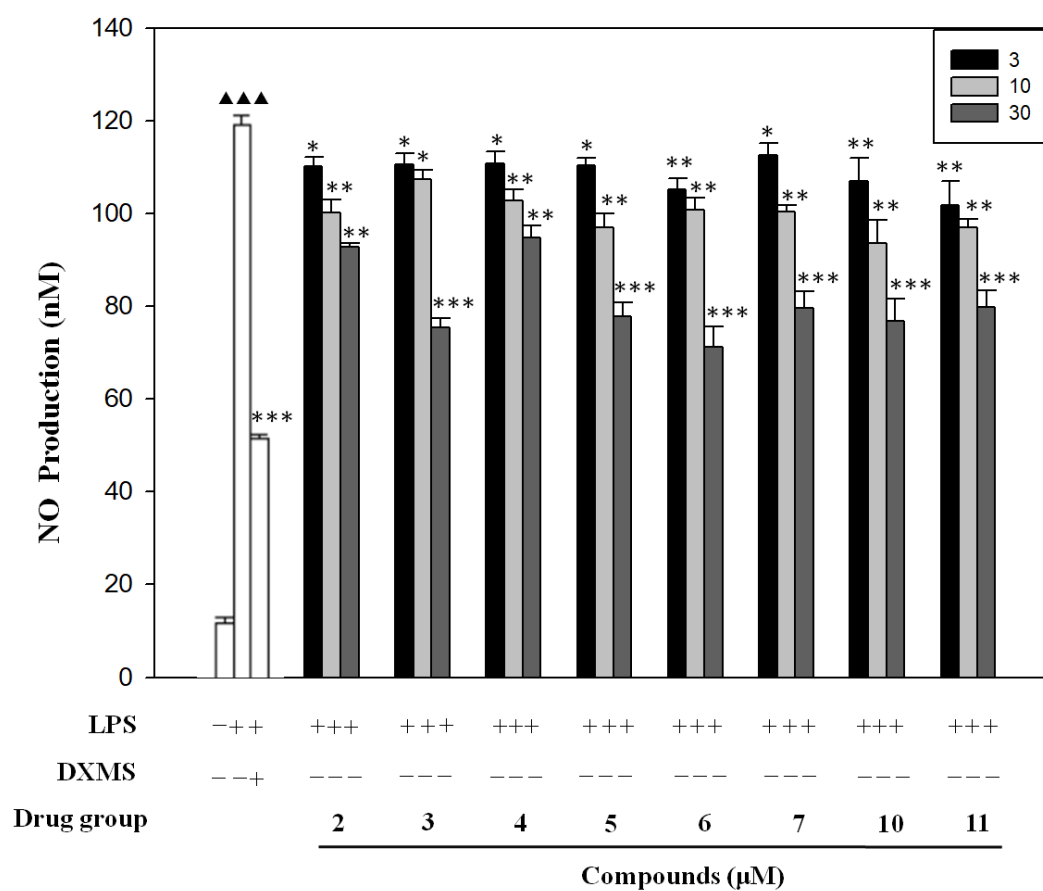


Figure S12. The effects of compounds **2–7** and **10-11** on NO production in LPS-stimulated RAW 264.7 cells.

DXMS (dexamethasone) was used as positive control. ▲▲▲ $p < 0.001$ vs normal untreated cells; * $p < 0.05$, ** $p < 0.01$, *** $p < 0.001$ vs LPS-stimulated cells.