SUPPLEMENTARY MATERIAL

Sesquiterpenes from Curcuma wenyujin with their inhibitory activities on nitric oxide production in RAW 264.7 cells

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One new sesquiterpene, 7α,11-epoxy-6α-hydroxy-carabrate-4,8-dione, along with ten known ones were isolated from the essential oil of Curcuma wenyujin Y. H. Chen et C. Ling. Their structures were established based on extensive spectroscopic analysis. The absolute configuration of compound 1 was determined by the CD analysis of the in situ formed [Rh2(OCOCF3)4] complex, and the CD data analysis based on the octane rule of cyclohexanone. The inhibitory effects of these sesquiterpenes on nitric oxide production in lipopolysaccharide-activated macrophages were also evaluated. Here, the biosynthesis pathway of the isolated compounds was proposed.

Keywords: Curcuma wenyujin; essential oil; sesquiterpenoids; nitric oxide; biosynthesis pathway
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Table S1. $^1$H and $^{13}$C-NMR data for compound 1$^a$.

| NO. | $\delta_c$ | $\delta_H$ ($J$ in Hz)      |
|-----|------------|-----------------------------|
| 1   | 25.0       | 0.66, ddd (8.4, 5.6, 5.1)   |
| 2   | 22.5       | 1.44, m                     |
|     |            | 1.66, m                     |
| 3   | 42.7       | 2.56, t (7.2)               |
| 4   | 208.4      |                             |
| 5   | 31.8       | 0.98, dd (5.1, 4.1)         |
| 6   | 70.3       | 4.09, d (4.1)               |
| 7   | 69.1       |                             |
| 8   | 205.2      |                             |
| 9   | 47.1       | 2.58, d (20.0)              |
|     |            | 2.60, d (20.0)              |
| 10  | 17.8       |                             |
| 11  | 64.2       |                             |
| 12  | 19.3       | 1.29, s                     |
| 13  | 20.4       | 1.02, s                     |
| 14  | 19.1       | 1.12, s                     |
| 15  | 29.7       | 2.08, s                     |

a: $^1$H-NMR spectra measured at 600 MHz, $^{13}$C-NMR spectra measured at 125 MHz; spectrum of compound 1 was obtained in DMSO-$d_6$. 
Table S2. Inhibitory effects of compounds 1-11 on NO production induced by LPS in macrophages.

| Compound | IC$_{50}$(mean ± SD) / μM |
|----------|--------------------------|
| 1        | 53.35±3.47               |
| 2        | 14.99±1.21               |
| 3        | >100                     |
| 4        | 59.06±3.26               |
| 5        | 98.48±7.09               |
| 6        | 81.35±6.68               |
| 7        | 80.76±4.89               |
| 8        | >100                     |
| 9        | 23.28±1.47               |
| 10       | 45.49±2.96               |
| 11       | 51.63±4.52               |
| Hydrocortisone$^b$ | 64.34±7.49 |

a: Inhibitory effects compounds 1-11 on NO production induced by LPS in RAW 264.7 macrophages.
b: Positive control.
Figure S1. Key HMBC correlations of compound 1.
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Figure S15. Inhibitory effect of γ-elemenolides on NO production induced by LPS in macrophages.

| NO. | Structure | IC$_{50}$(mean ± SD) / μM |
|-----|-----------|--------------------------|
| 1$^a$ | ![Structure](image1.png) | 14.99±1.21 |
| 2$^b$ | ![Structure](image2.png) | 26.0 |
| 3$^c$ | ![Structure](image3.png) | 69.98 ± 6.21 |

a: compound 2 which were isolated from *Curcuma wenyujin*.  
b: compound 9 which were isolated from *Curcuma wenyujin*. (Lou et al. 2010)  
c: compound 6 which were isolated from *Curcuma phaeocaulis*. (Ma et al. 2015)  
d: Inhibitory effects compounds on NO production induced by LPS in RAW 264.7 macrophages.
Figure S16. Analysis based on the octane rule of cyclohexanone of 1.